Asynchronously Parallel Optimization Solver for Finding Multiple Minima

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Problem setup

Want to find distinct, high-quality minima for the problem

$$\begin{aligned} &\underset{x \in \mathbb{R}^n}{\text{minimize}} \; f(x) \\ &\text{subject to: } x \in \mathcal{D}, \end{aligned}$$

when $\mathcal{D}$ is compact, c concurrent evaluations of f are possible, and relatively little is known about f a priori.

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- Derivatives of f may or may not be available
- c is fairly small
- Evaluating f is expensive
- High-quality can be measured by more than the objective

Motivation

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Initial approaches

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  - Genetic Algorithm
  - Simulated Annealing
  - Particle Swarm
  - Ant Colony Optimization
  - Bee Colony Optimization
  - Cuckoo Search
  - Bacterial Colony Optimization
  - Grey Wolf Optimization
  - Firefly Optimization
  - Harmony Search
  - River Formation Dynamics

Global DFO

Theorem (Törn and Žilinskas, *Global Optimization*, 1989)

An algorithm converges to the global minimum of any continuous f on a domain $\mathcal{D}$ if and only if the algorithm generates iterates that are dense in $\mathcal{D}$.

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+ Get to use (more developed) local optimization routines.
  - least-squares objectives, nonsmooth objectives, (un)relaxable constraints, and more
+ Increased opportunity for parallelism
  - objective, local solver, and global solver
- Can require many sequential evaluations for the local solver

Where to start?

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$\hat{x} \in \mathcal{S}_k$

(S2) $\nexists x \in \mathcal{S}_k$ *with* $[\|\hat{x} - x\| \leq r_k$ *and* $f(x) < f(\hat{x})]$

(S3) $\hat{x}$ *has not started a local optimization run*

(S4) $\hat{x}$ *is at least* μ *from* $\partial\mathcal{D}$ *and* ν *from known local minima*

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APOSMM: (S1)–(S4), (L1)–(L6)

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(L5) $\hat{x}$ is not in an active local optimization run and has not been ruled stationary

(L6) $\exists r_k$-descent path in $\mathcal{H}_k$ from some $x \in \mathcal{S}_k$ satisfying (S2-S4) to $\hat{x}$

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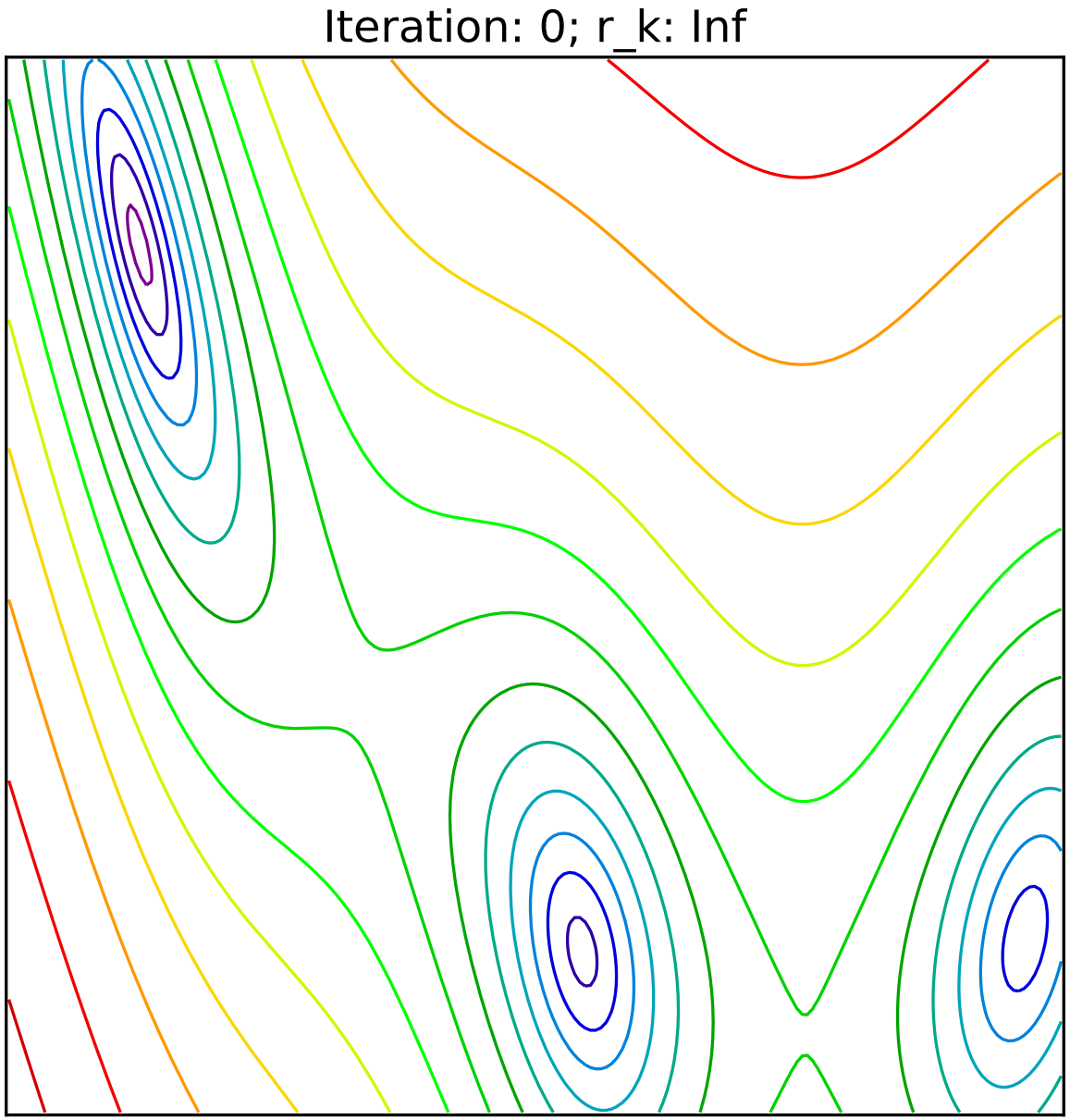

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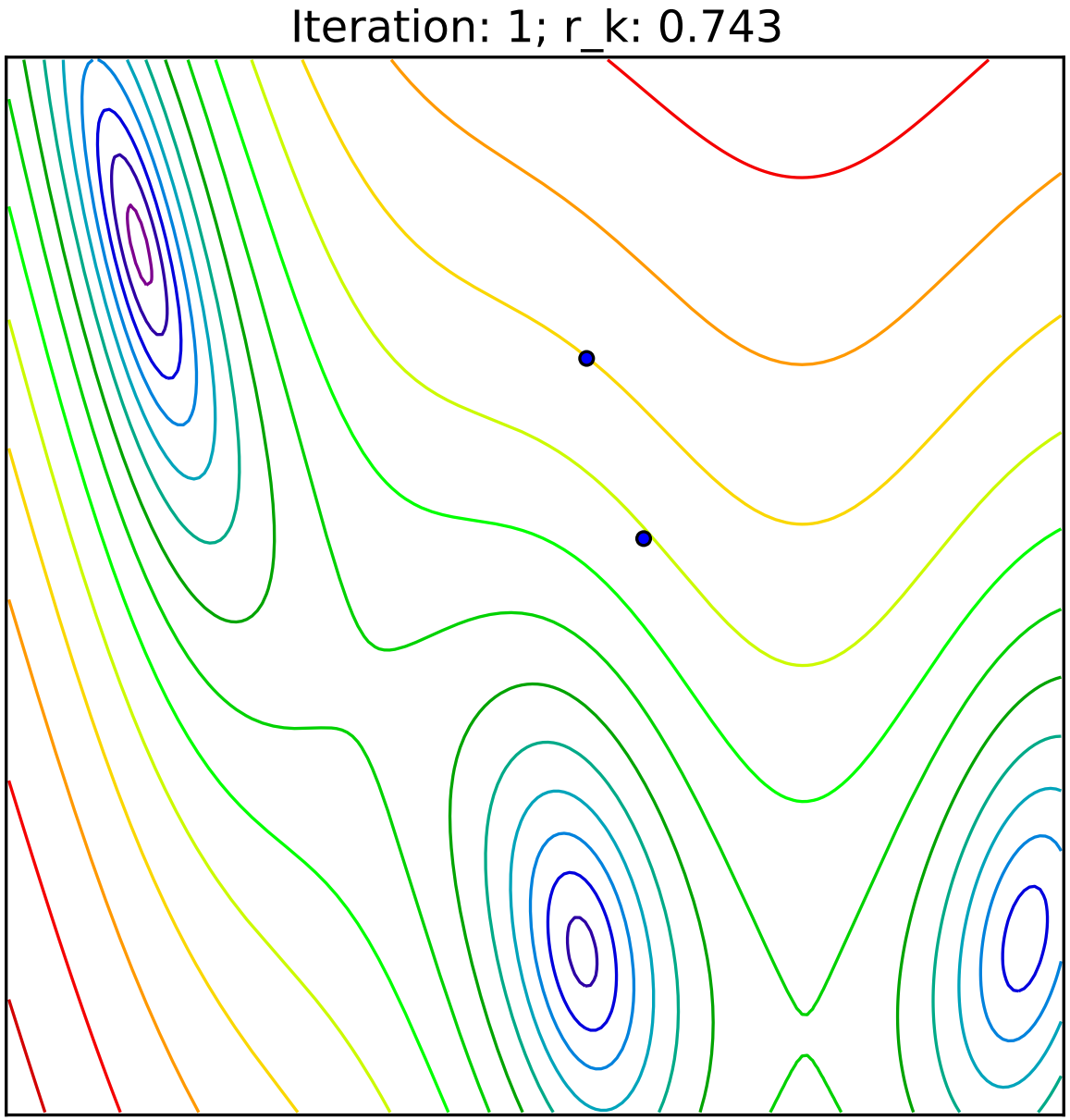

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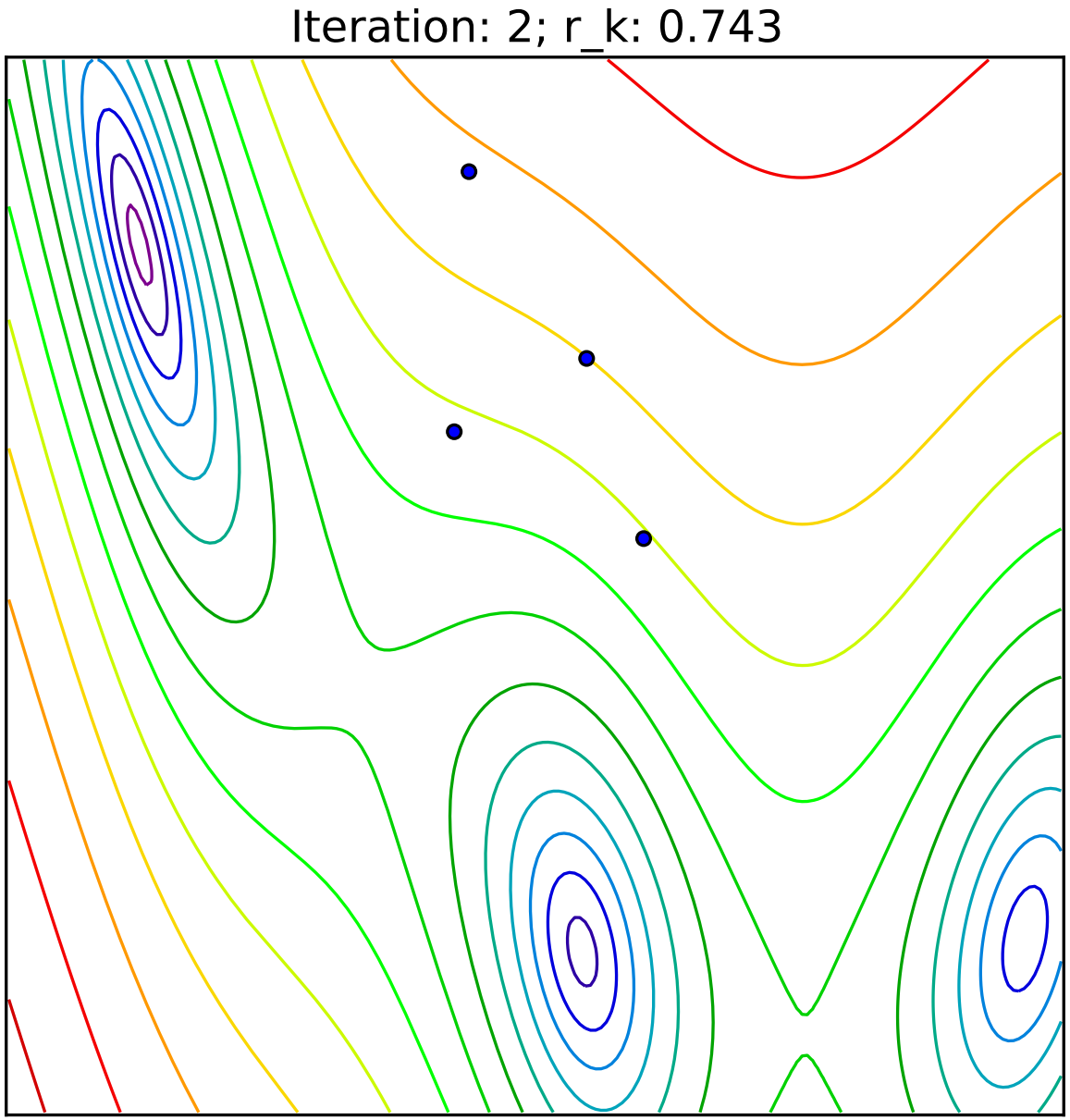

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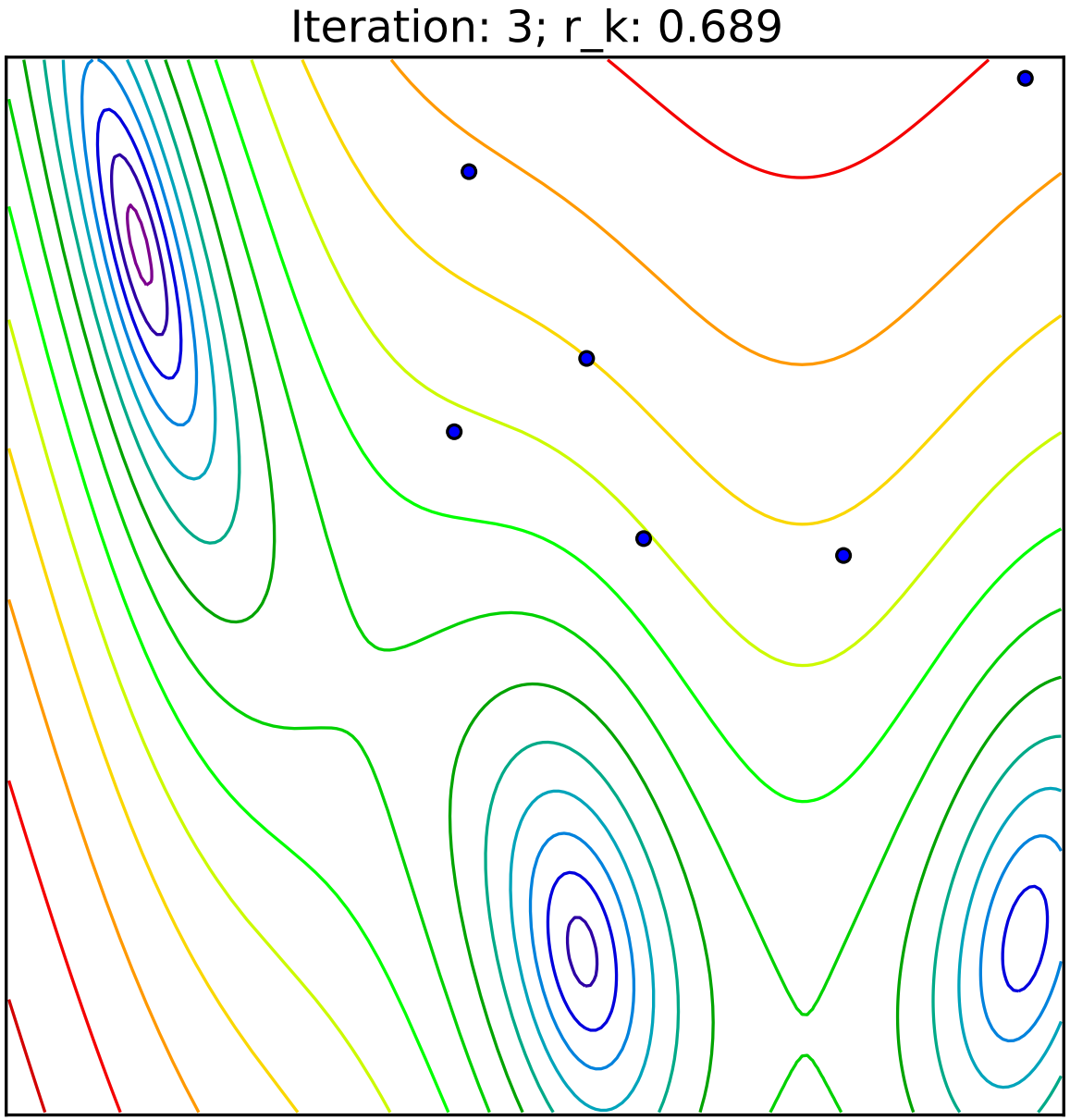

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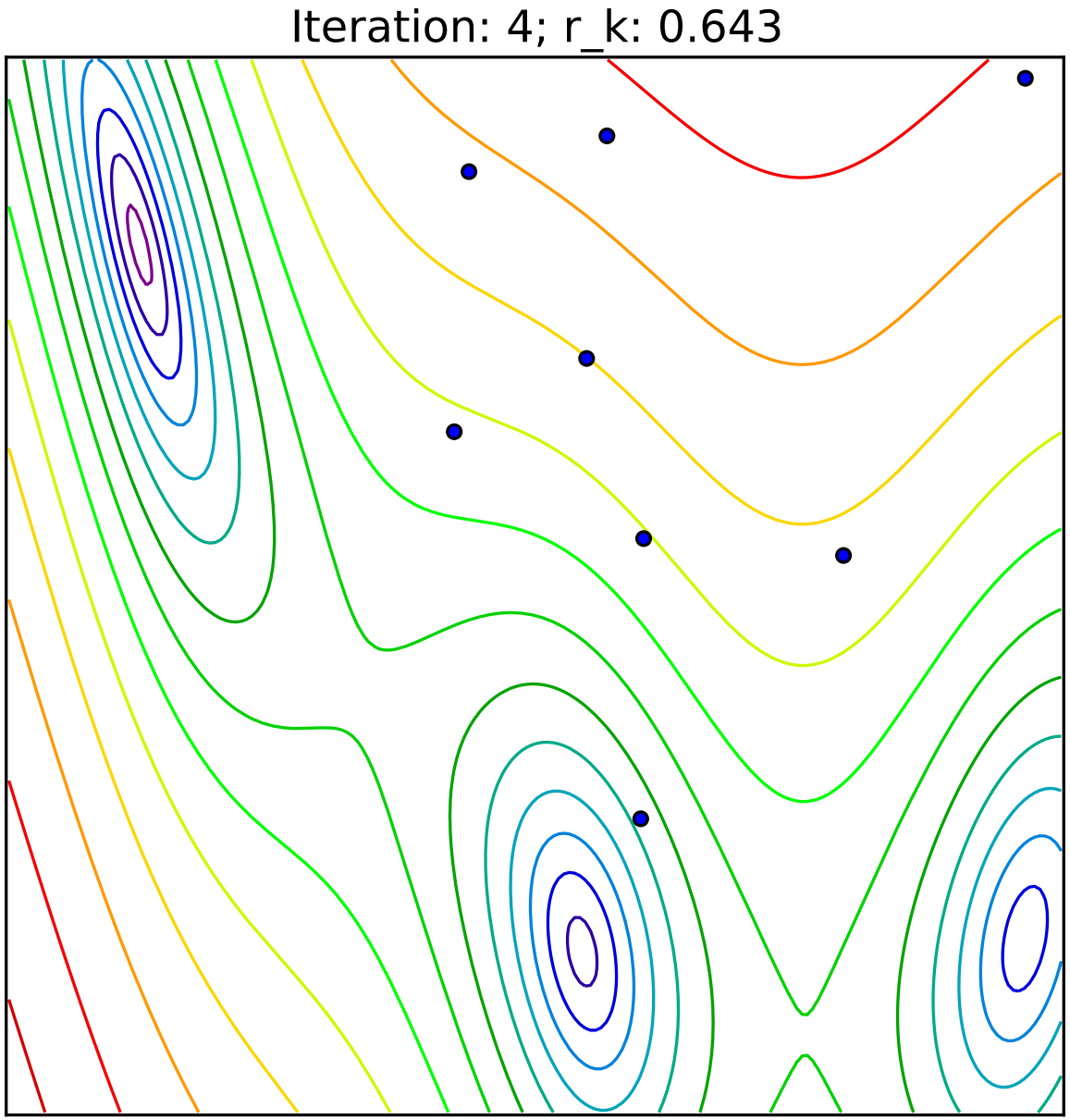

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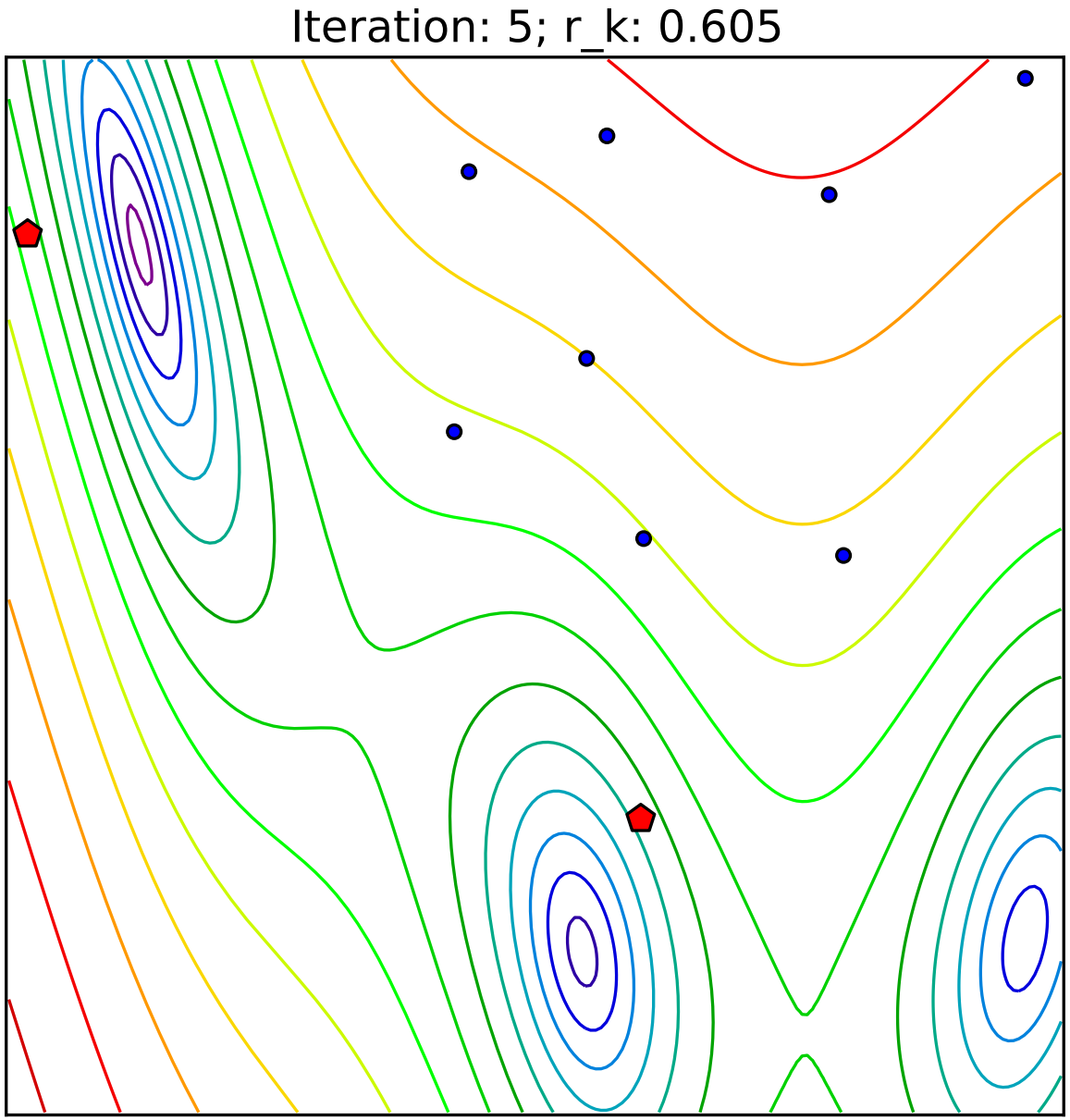

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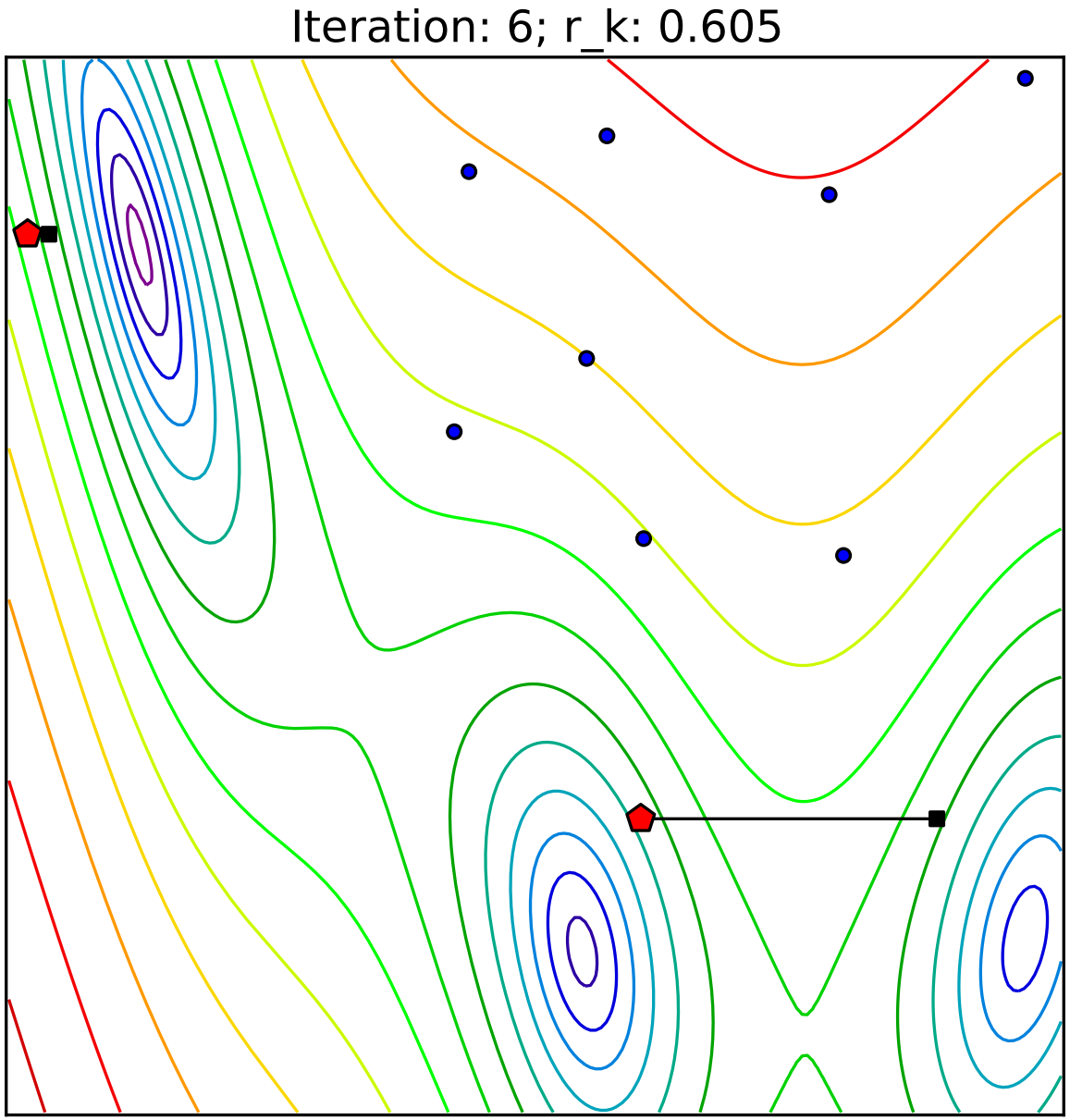

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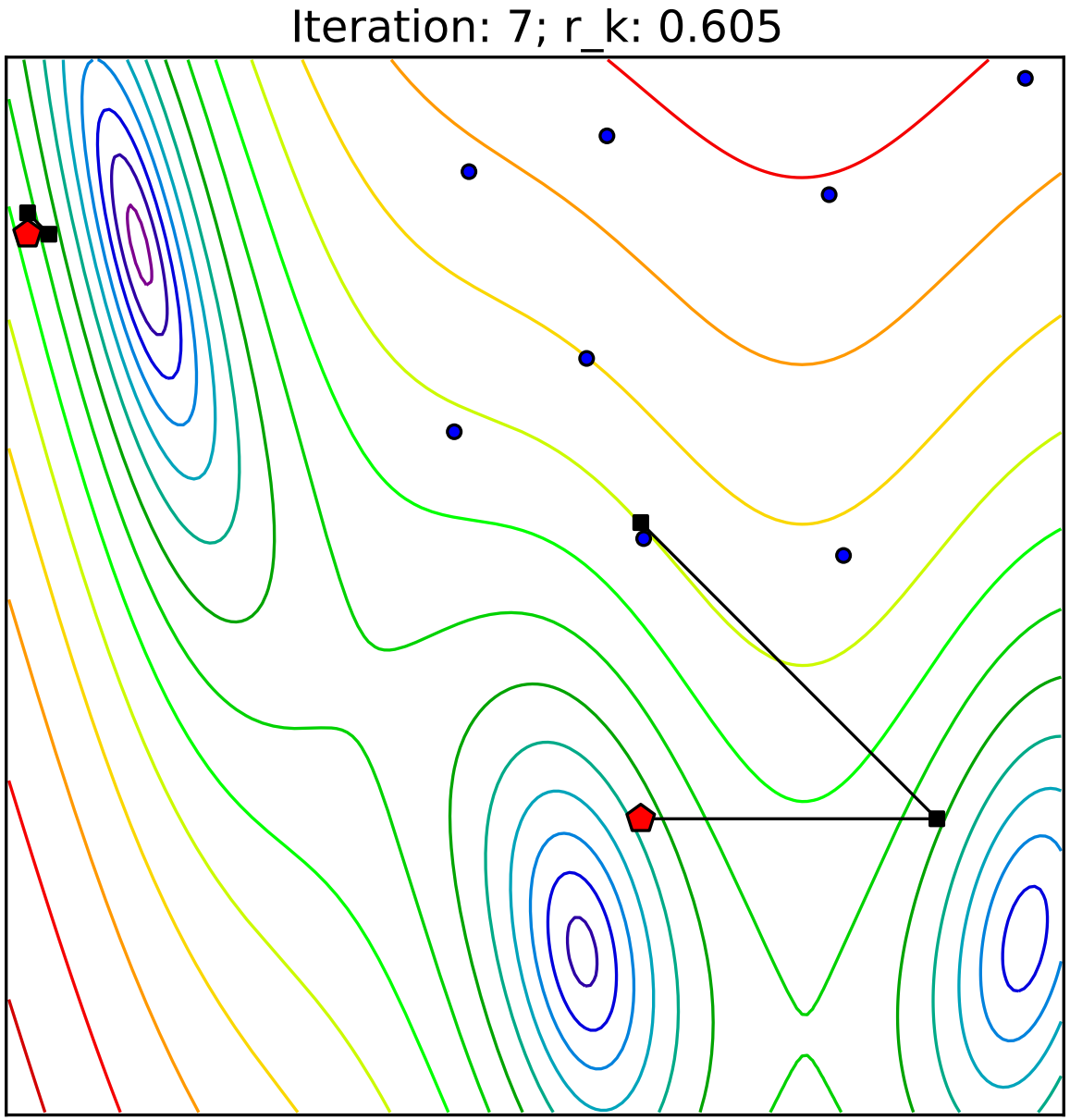

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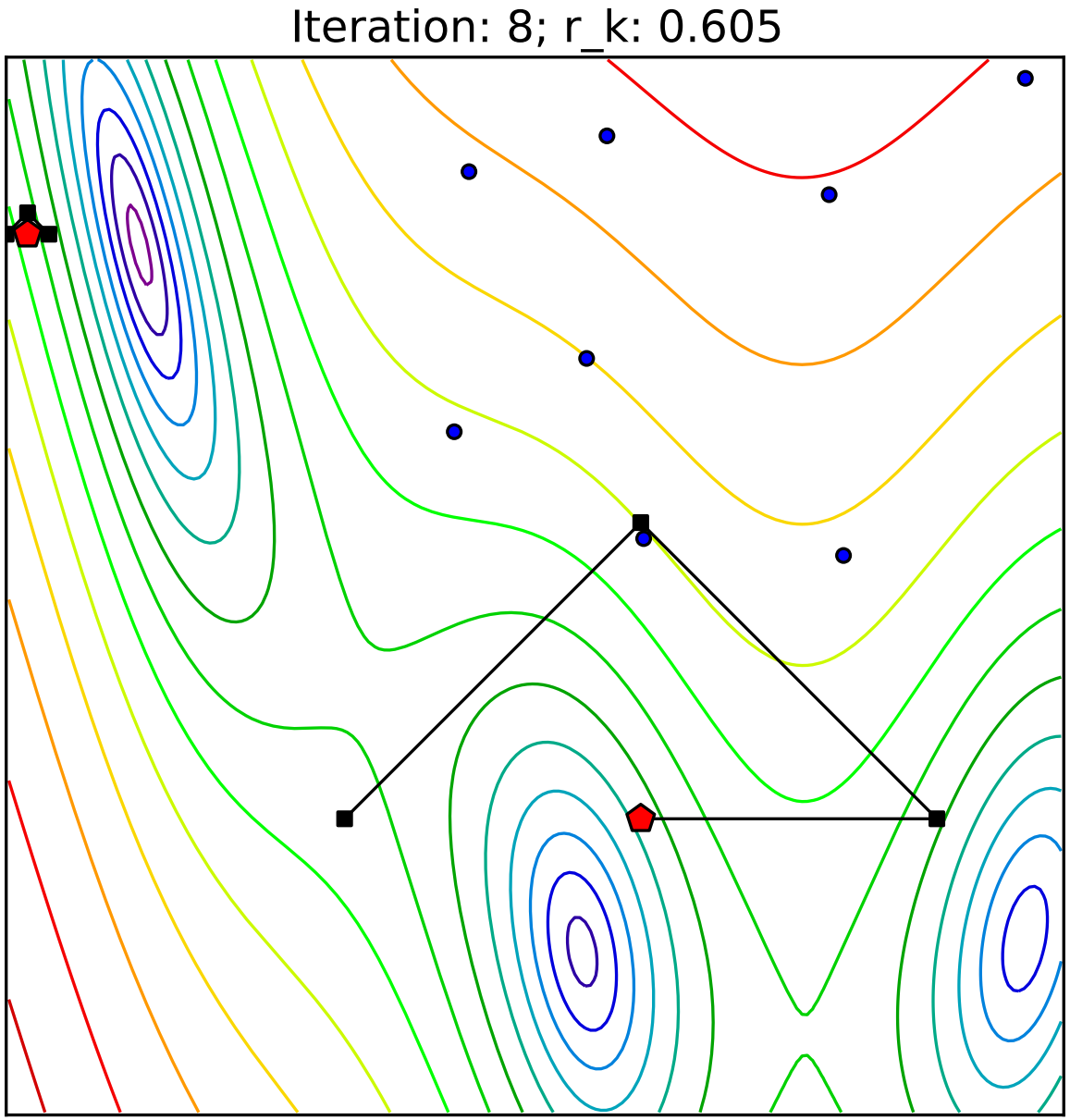

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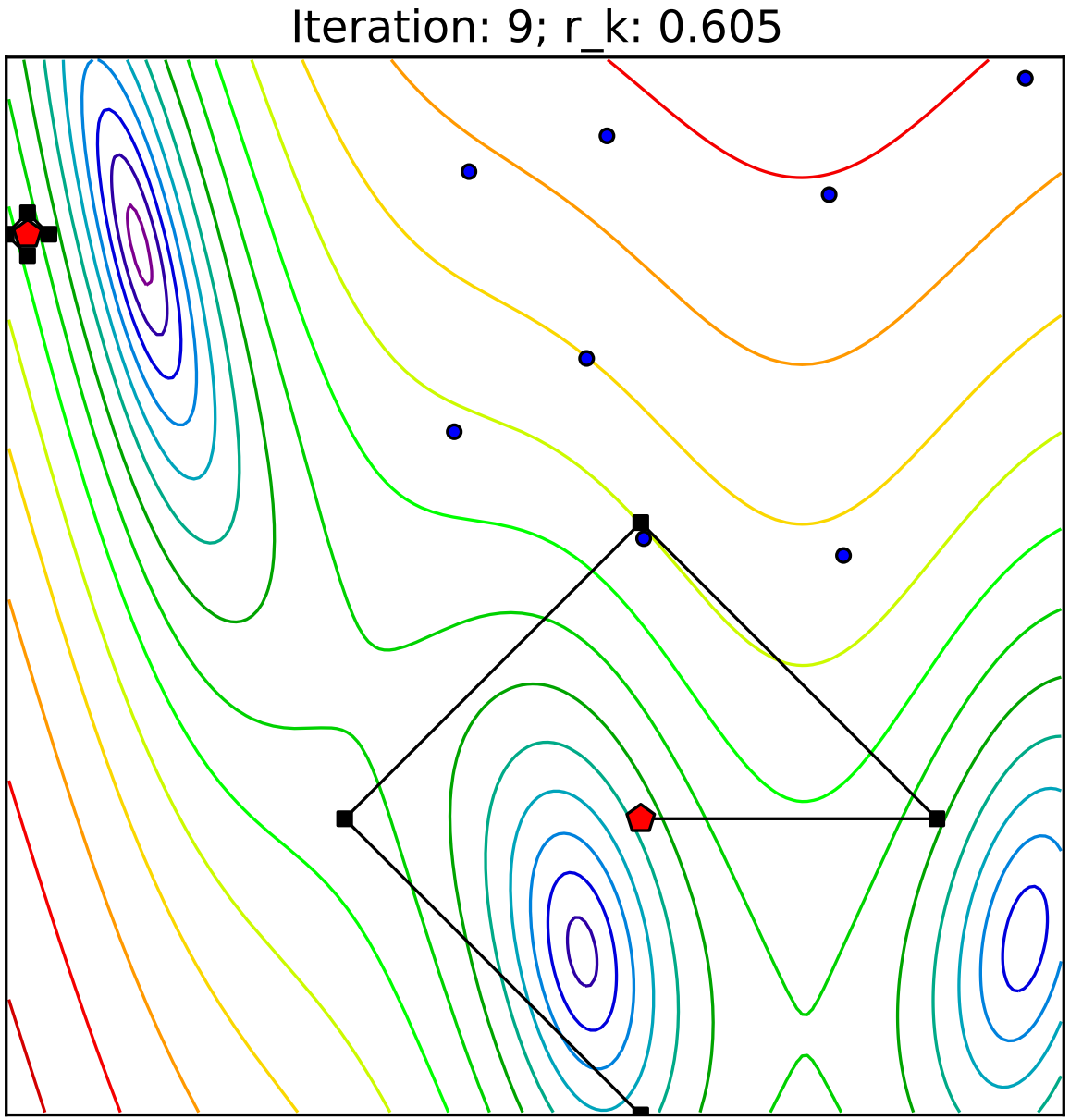

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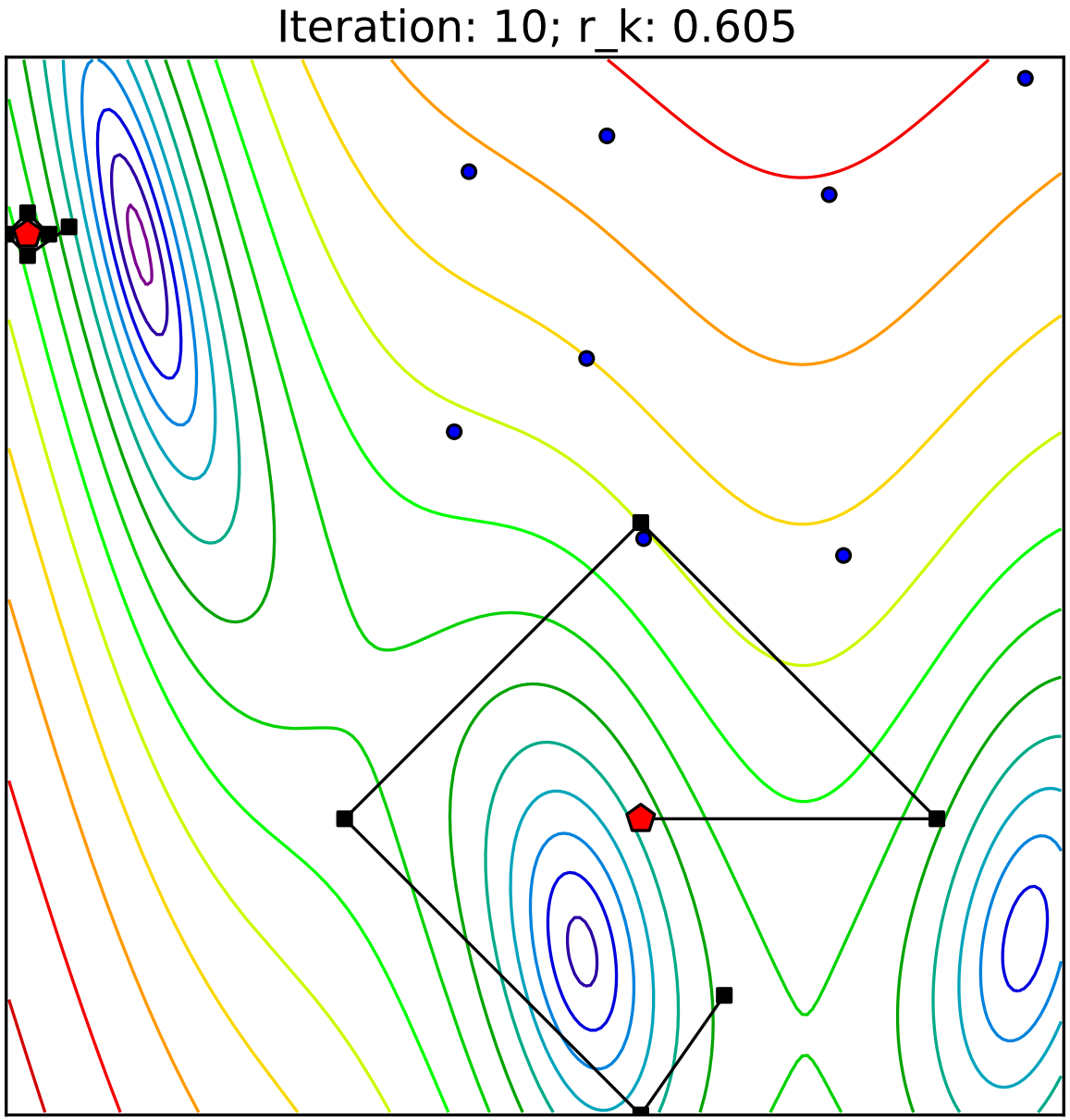

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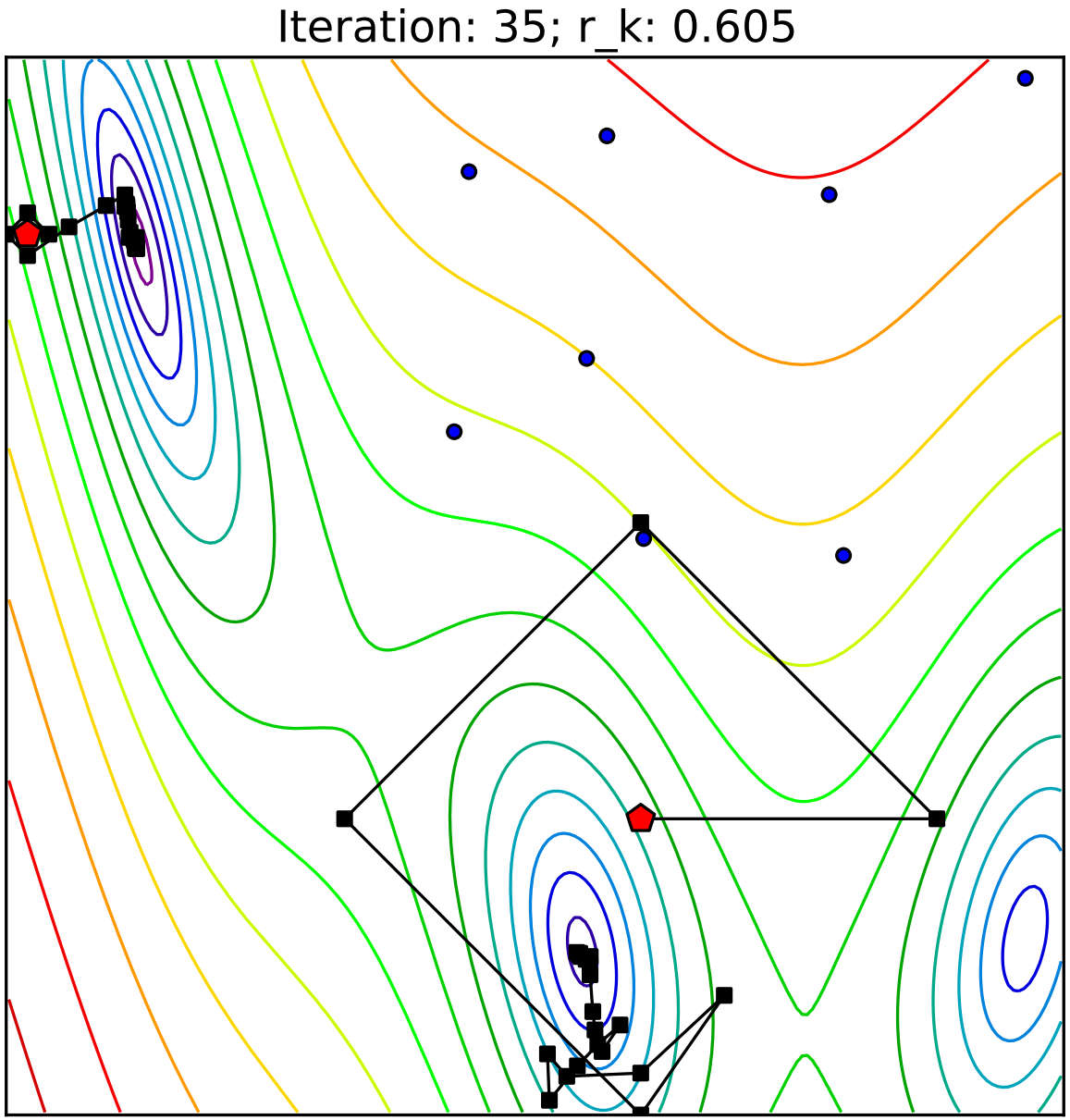

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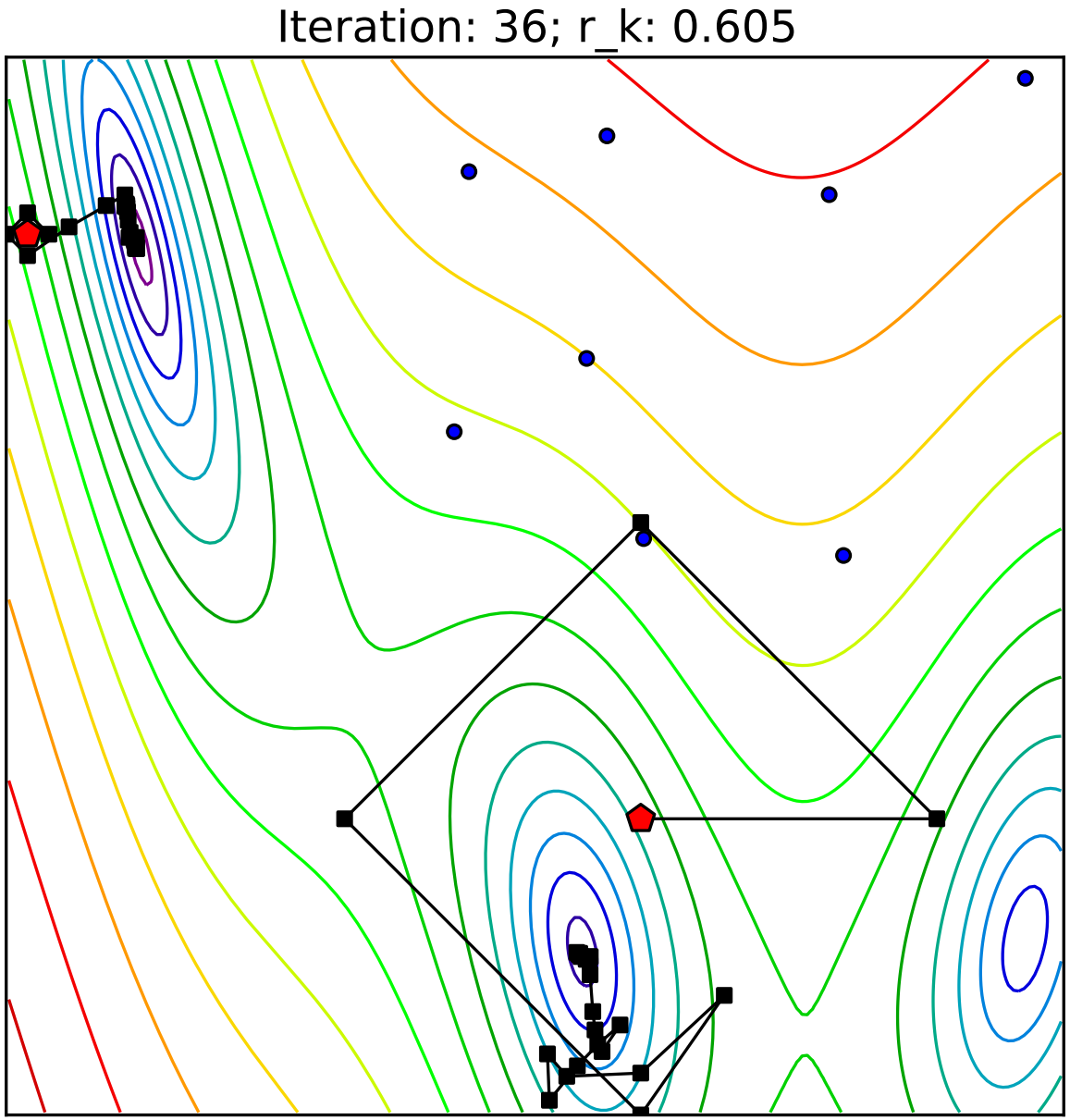

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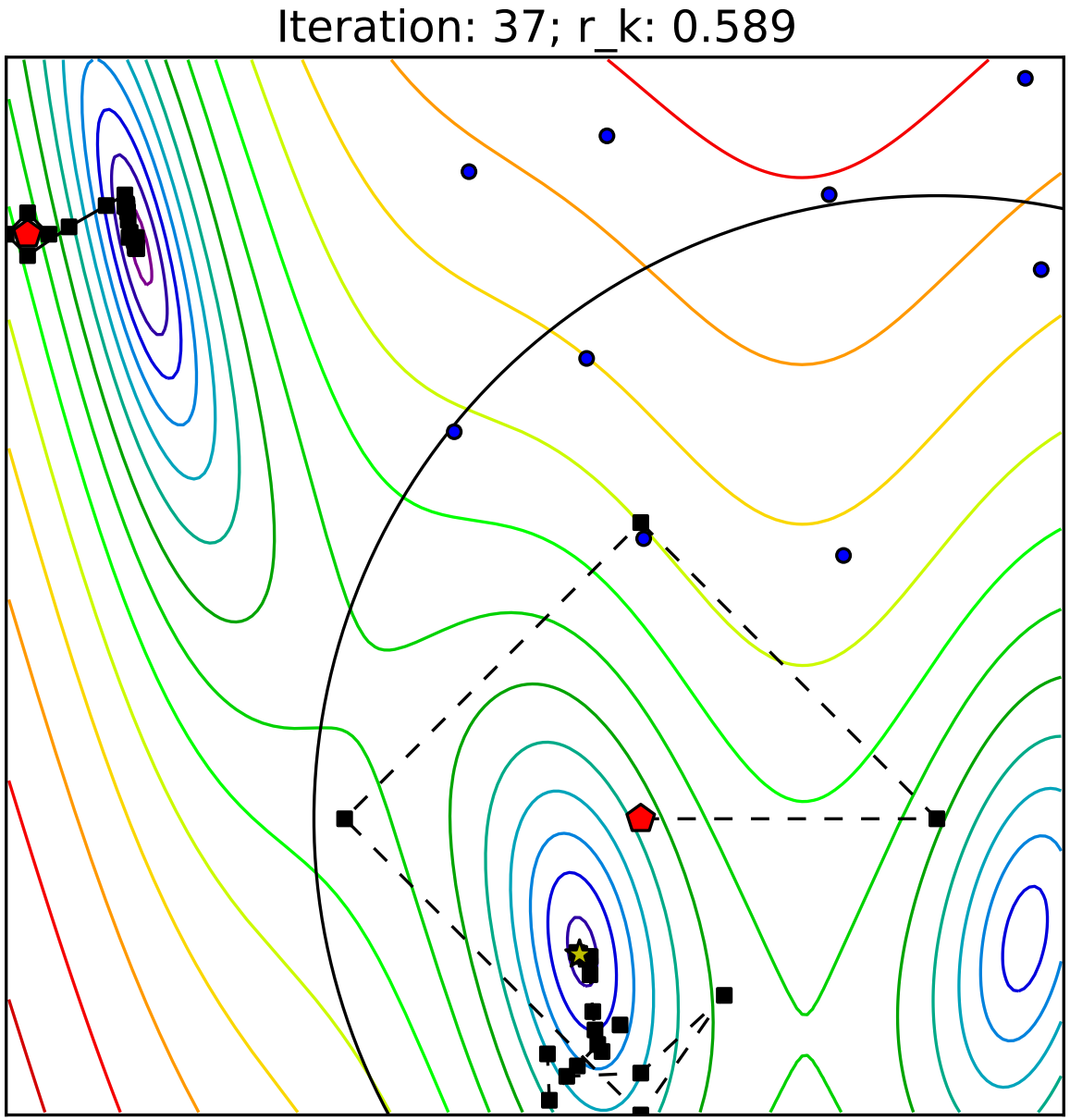

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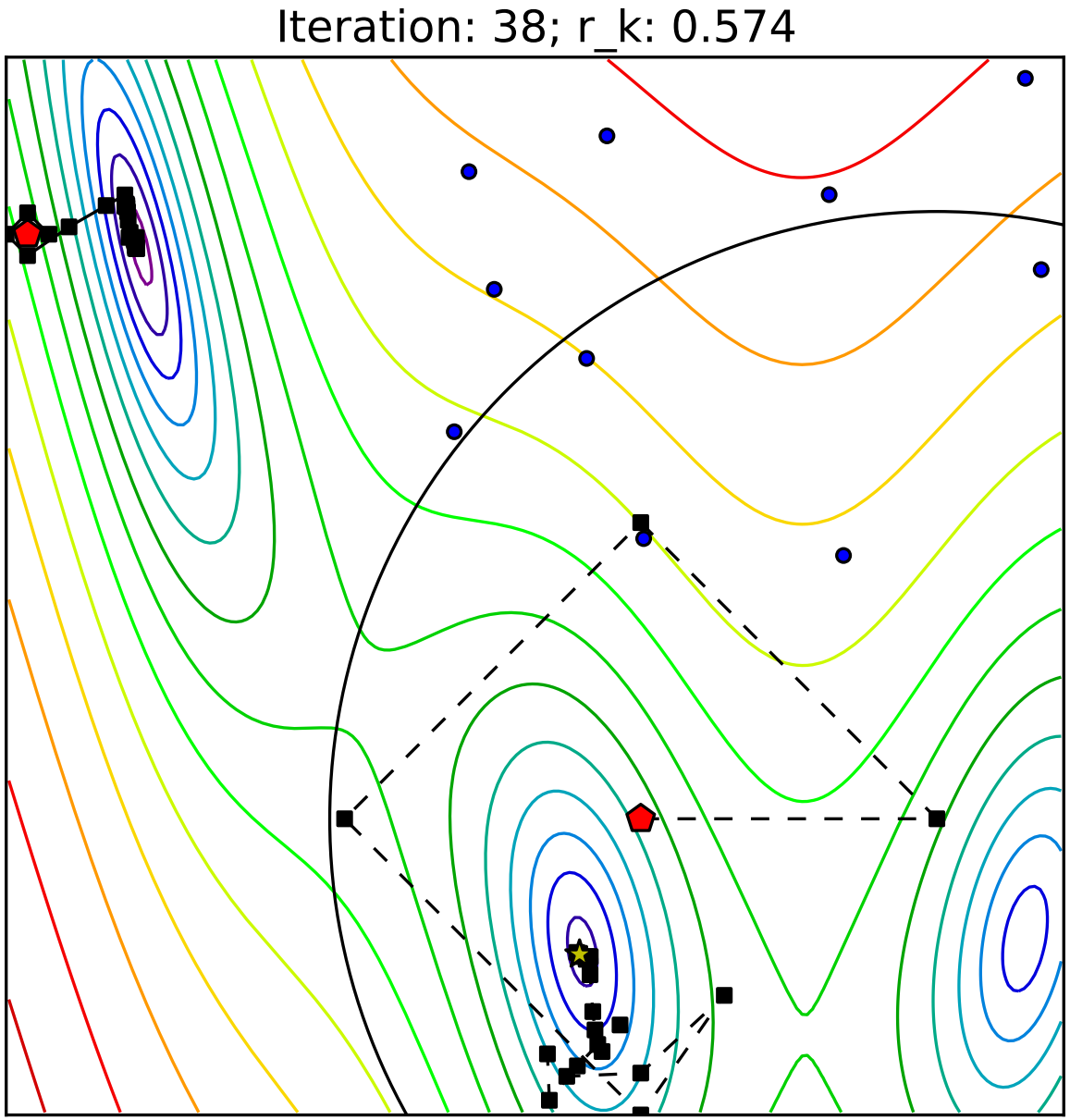

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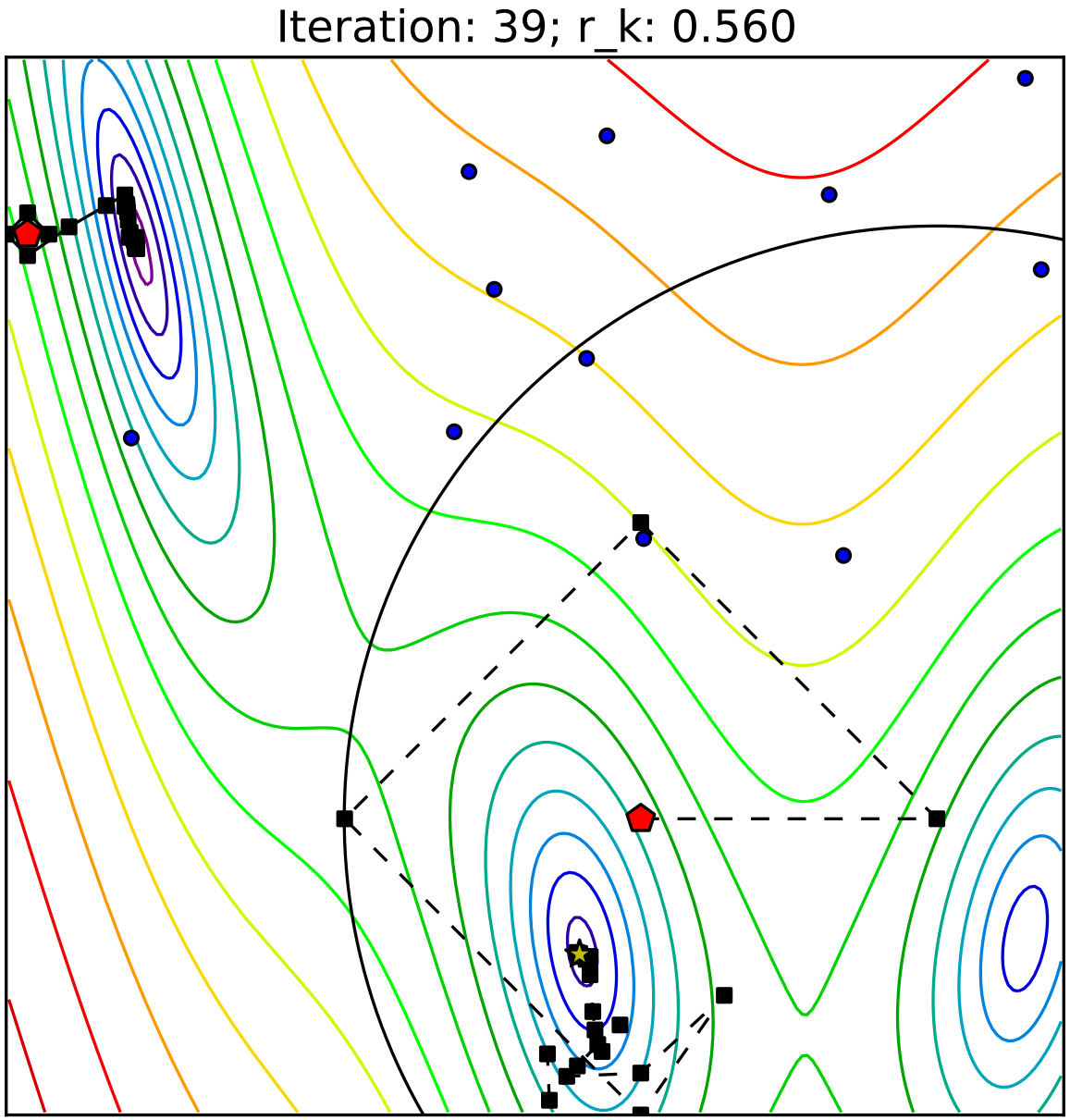

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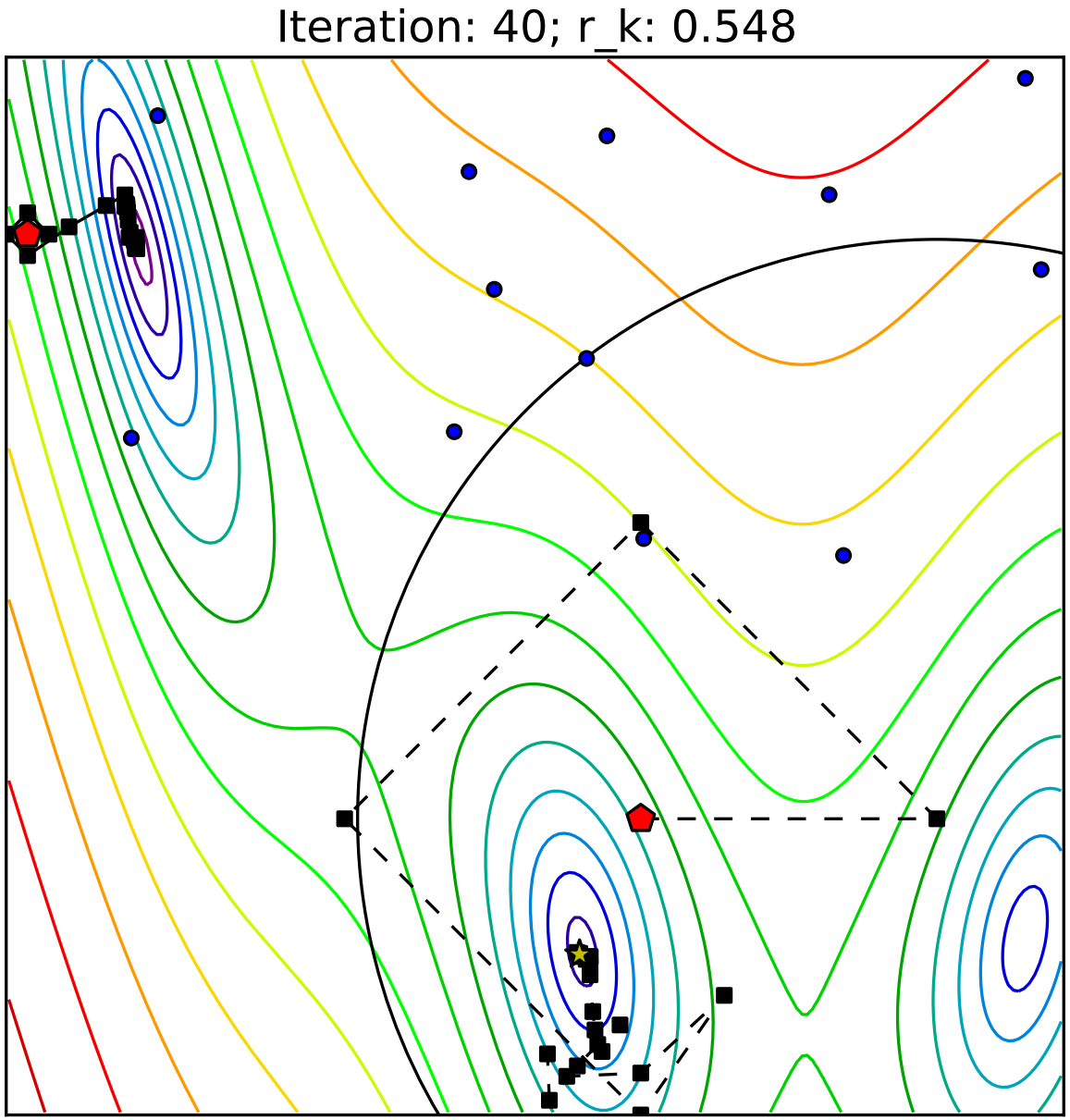

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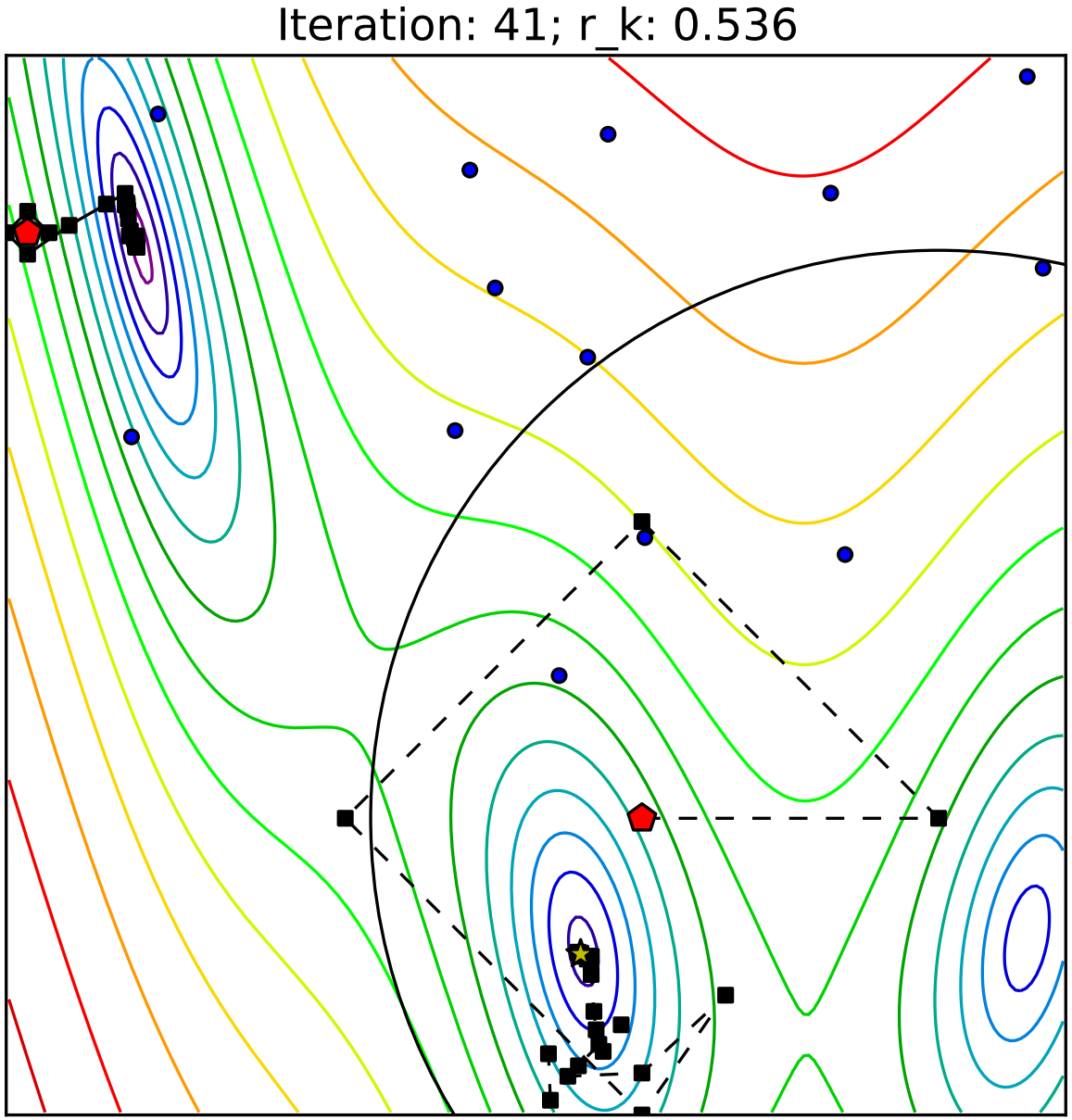

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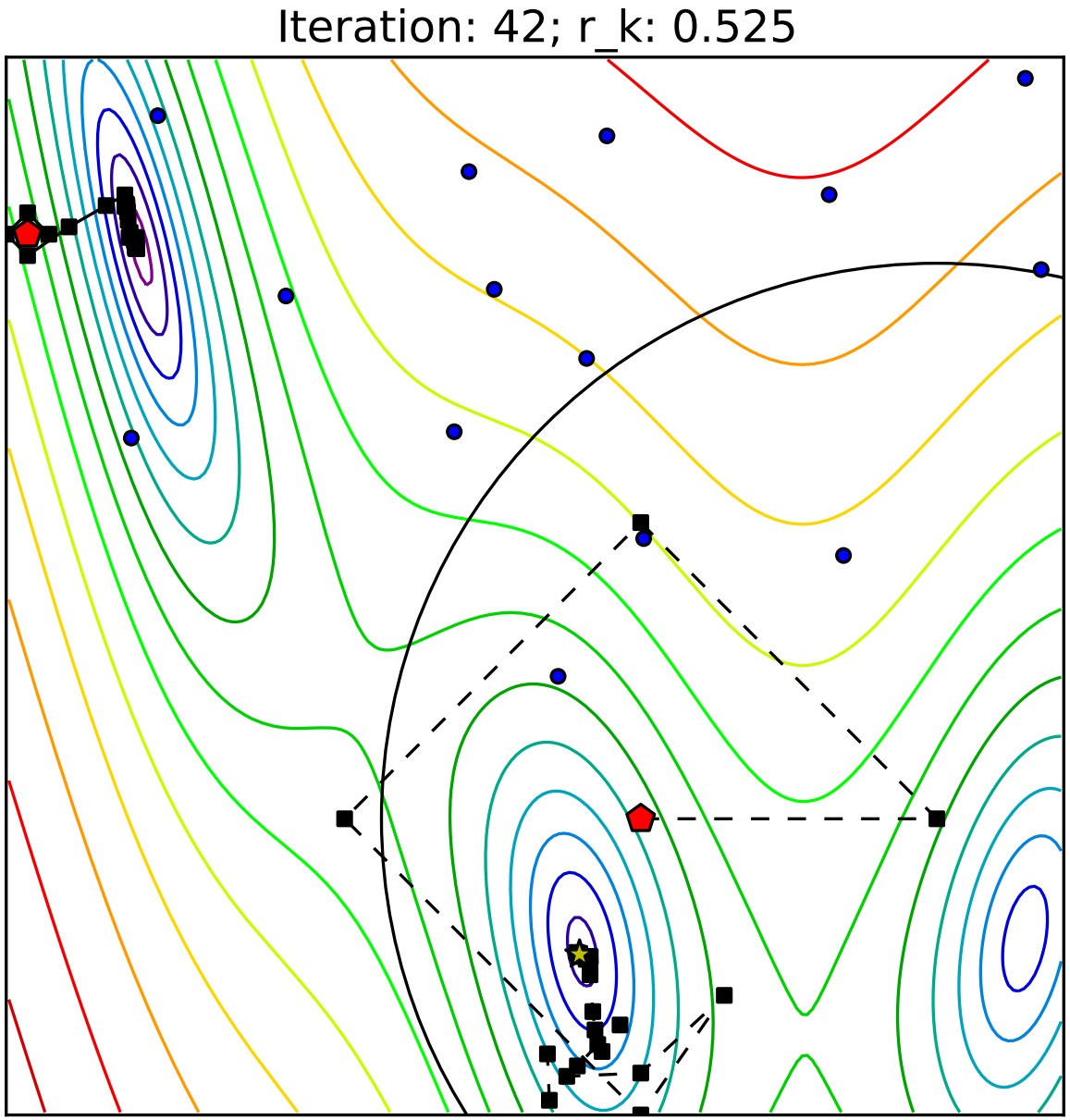

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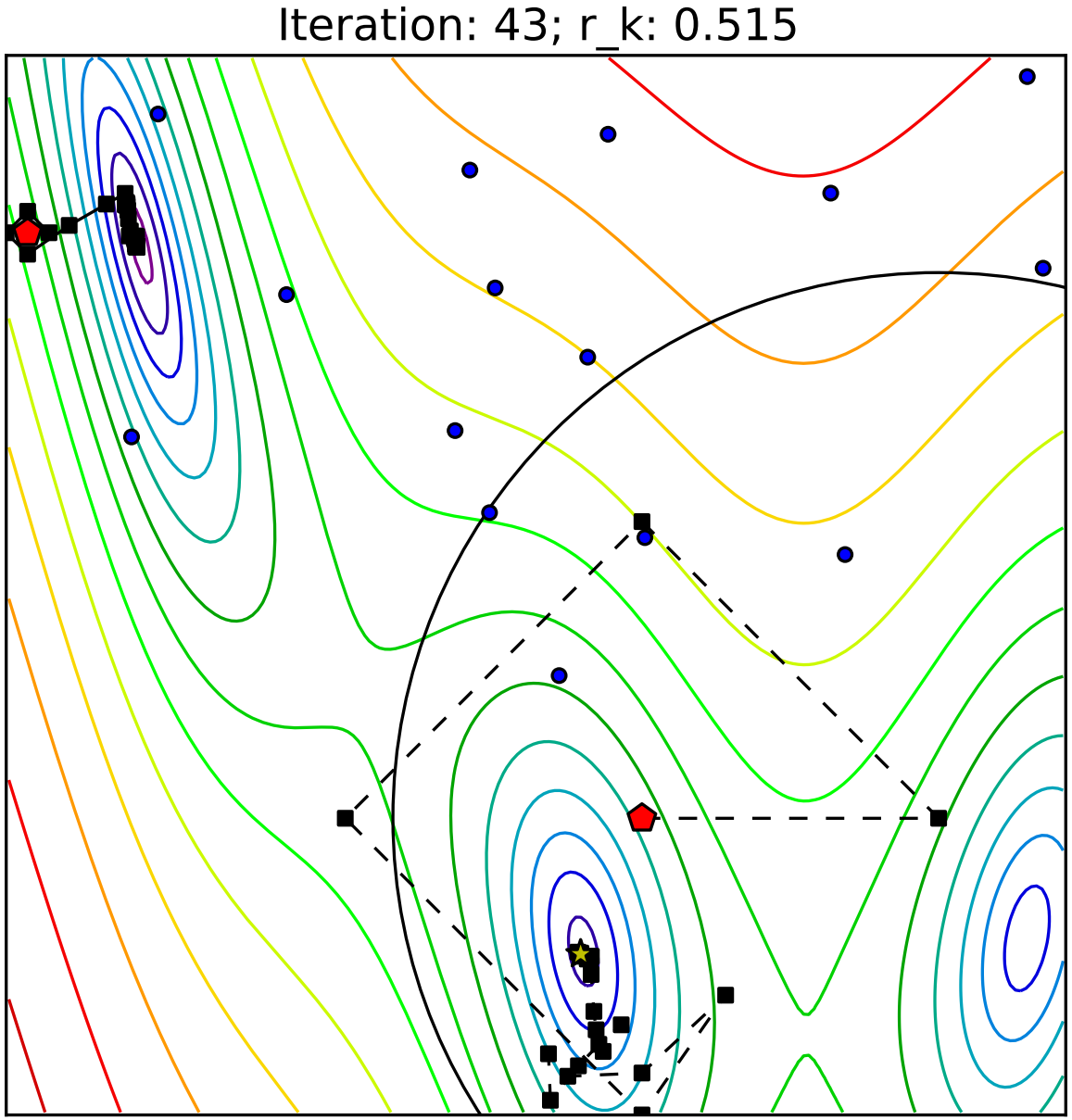

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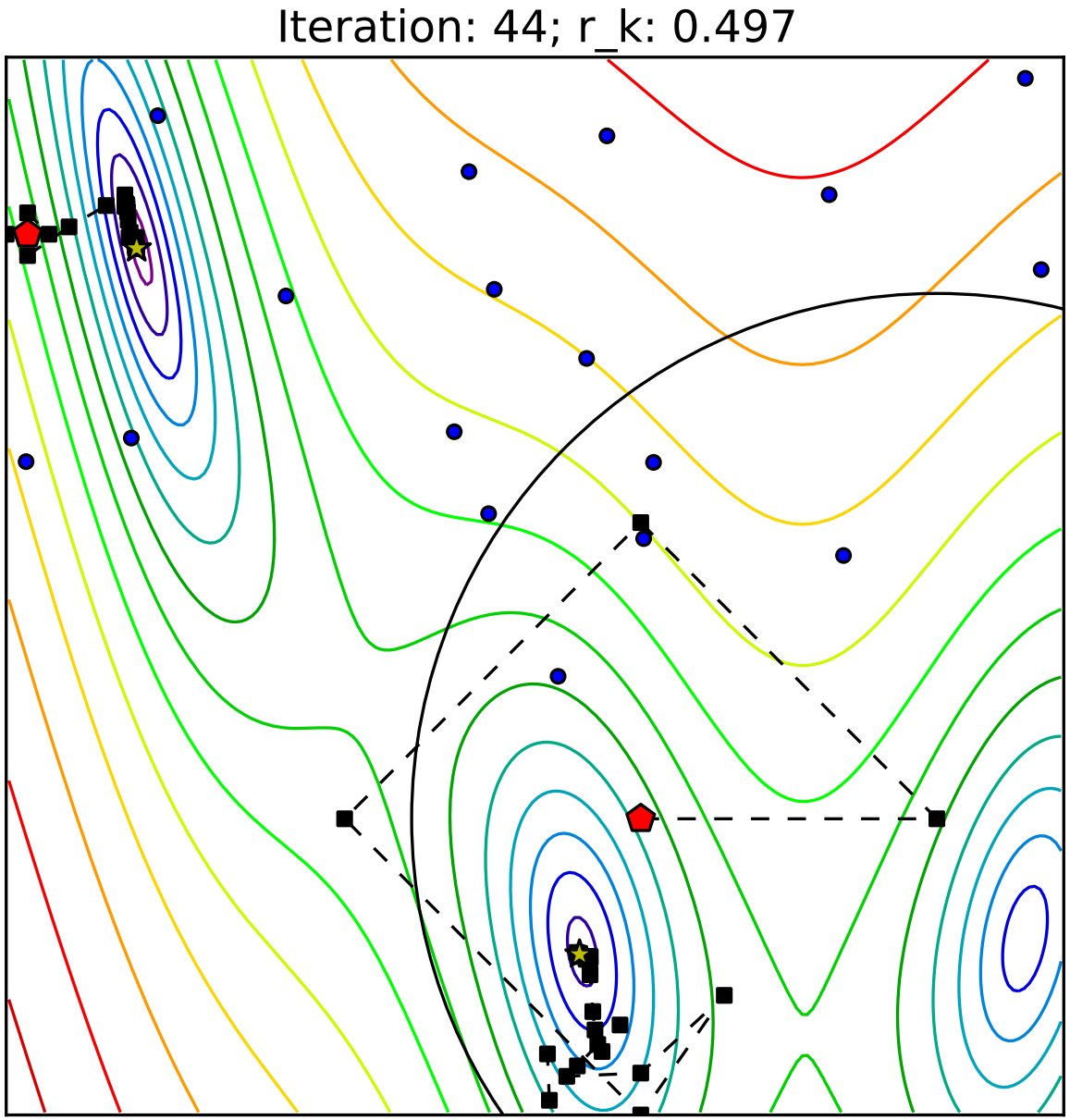

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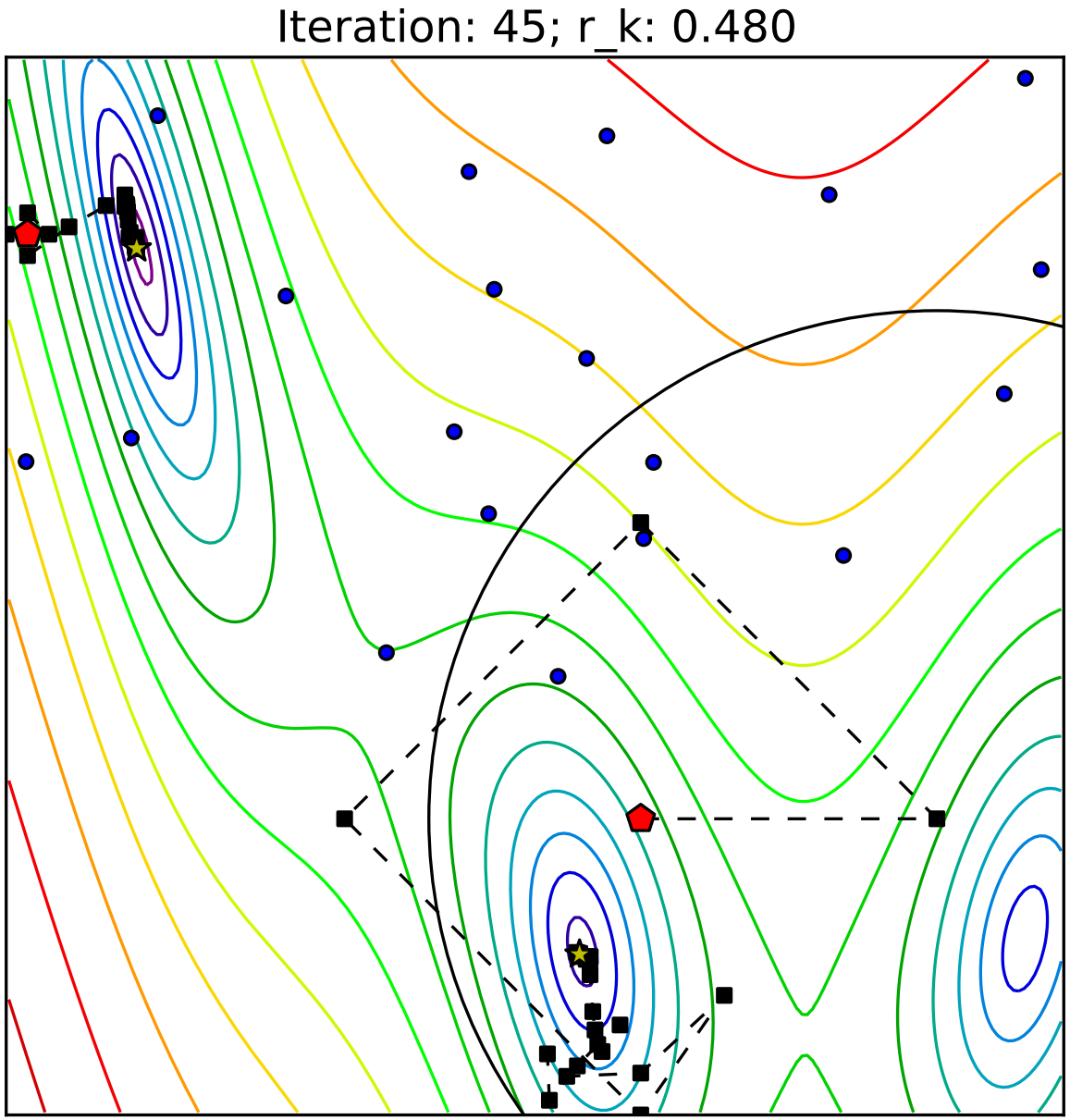

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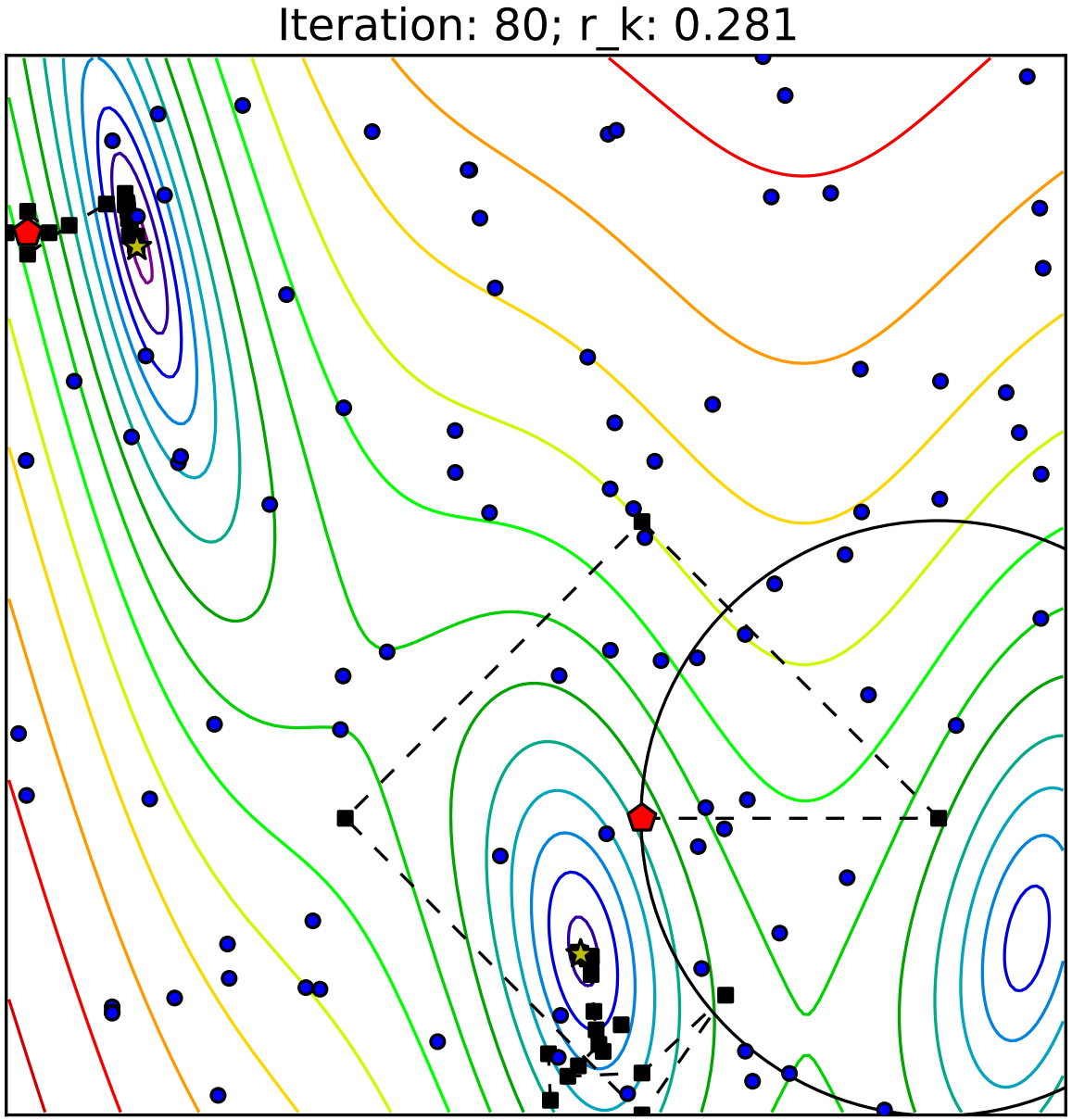

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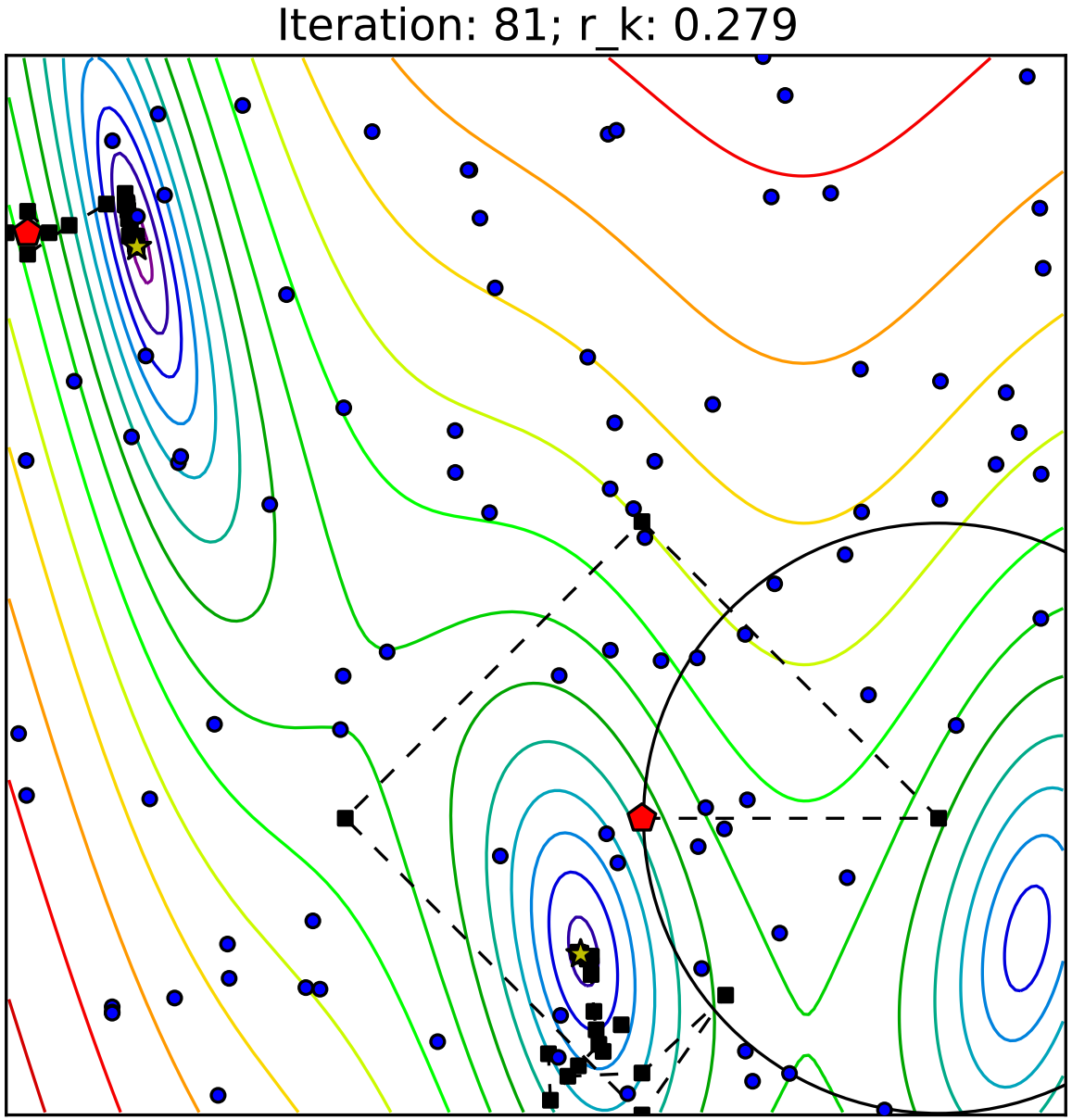

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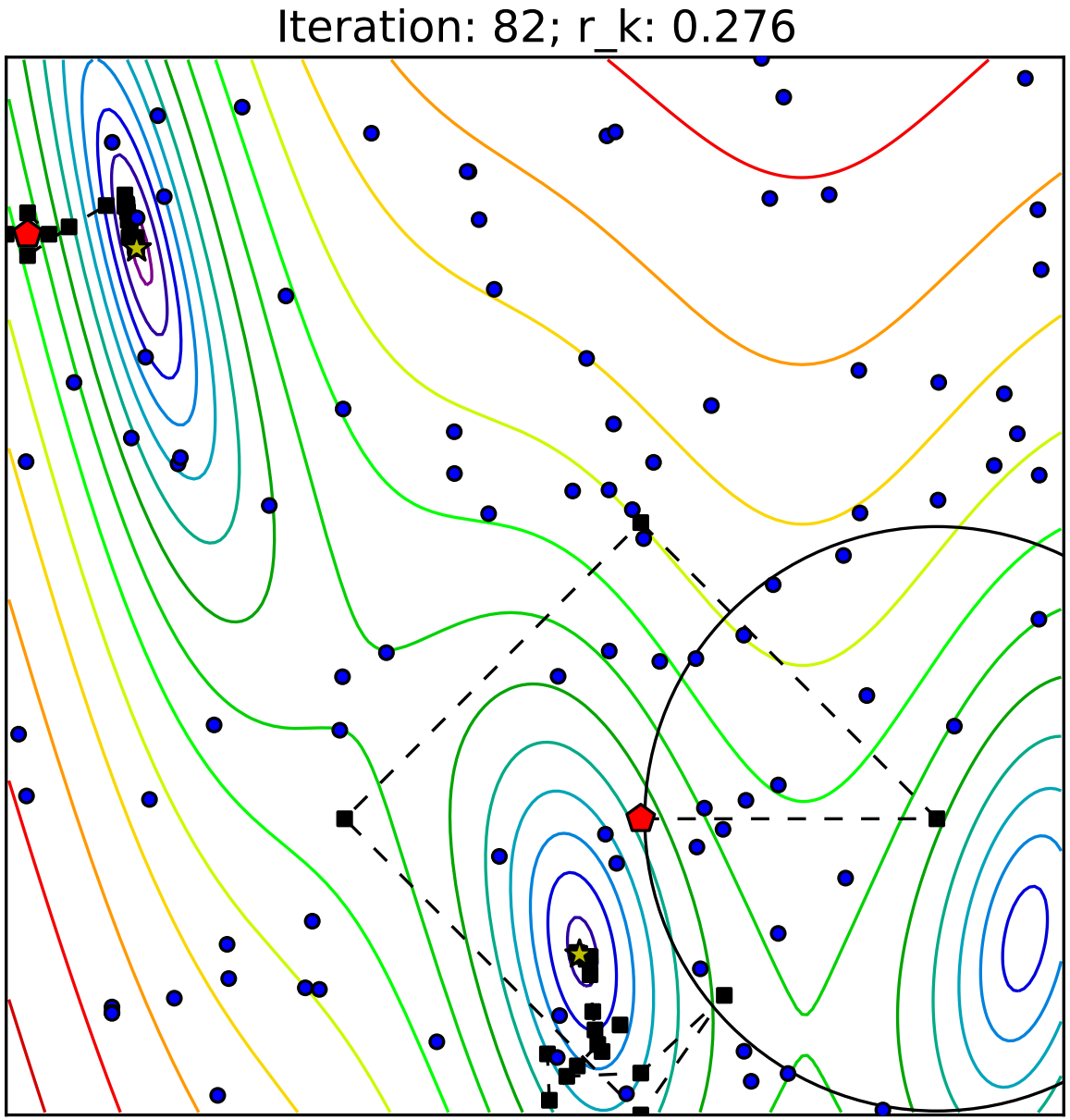

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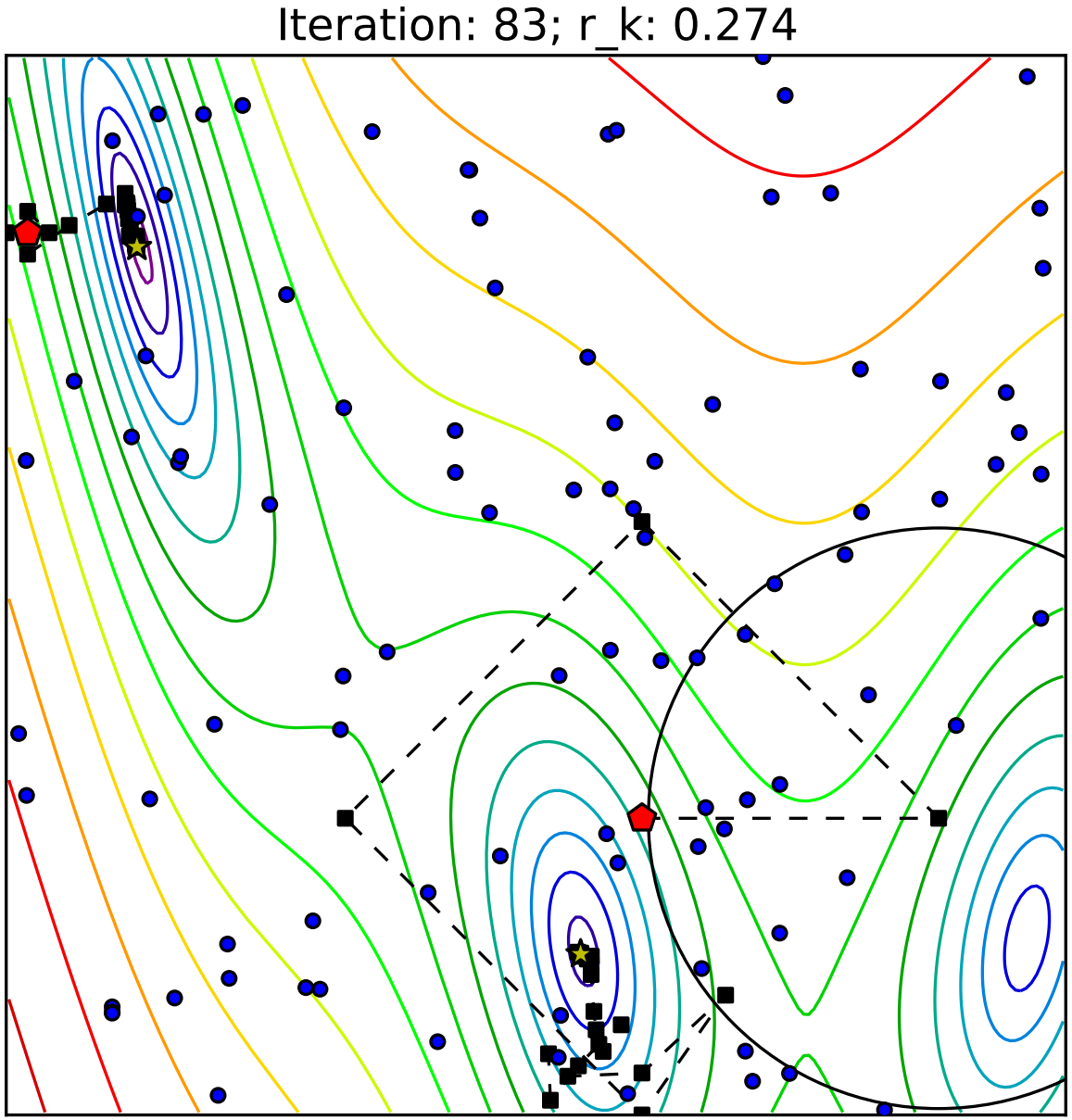

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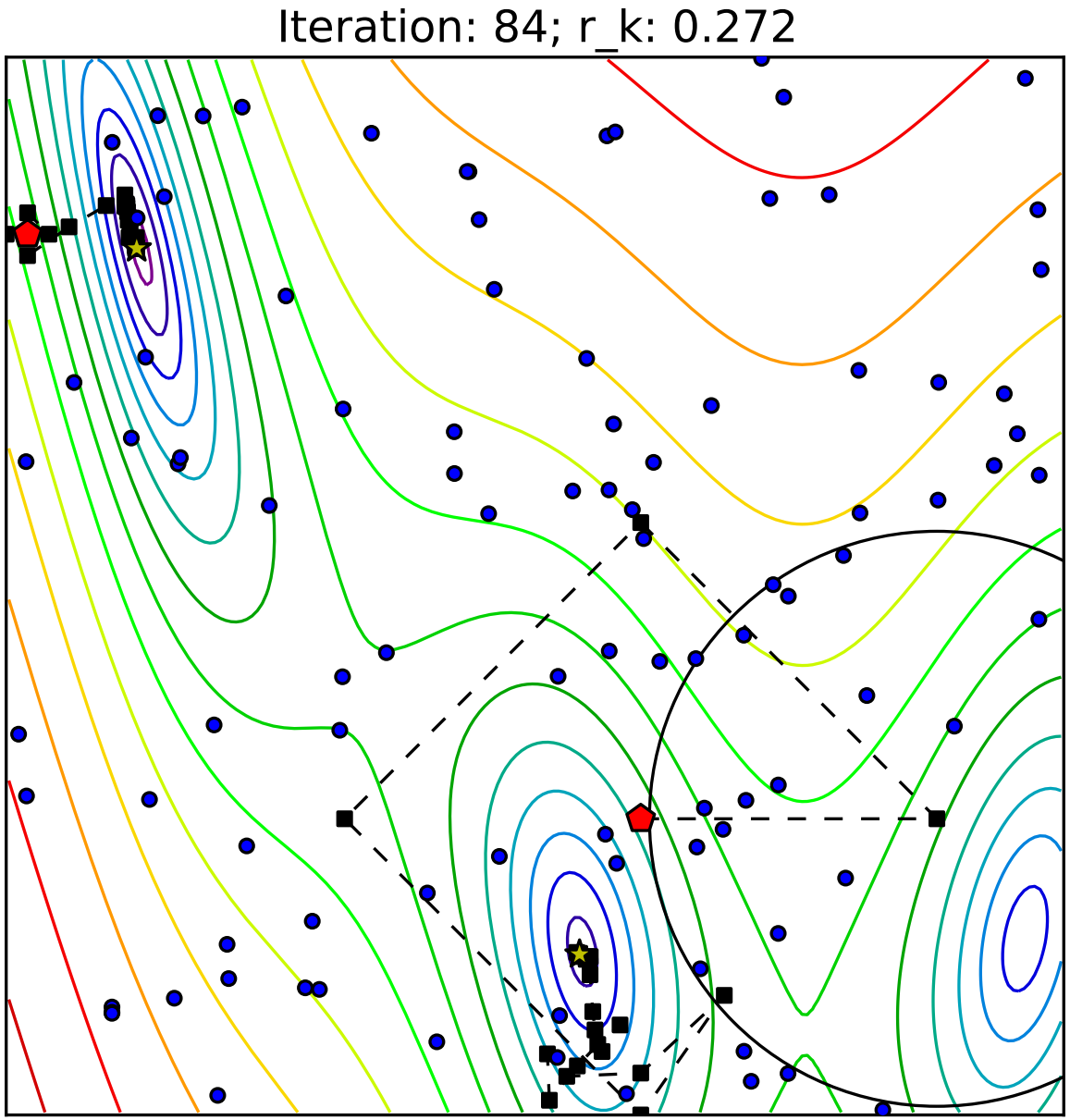

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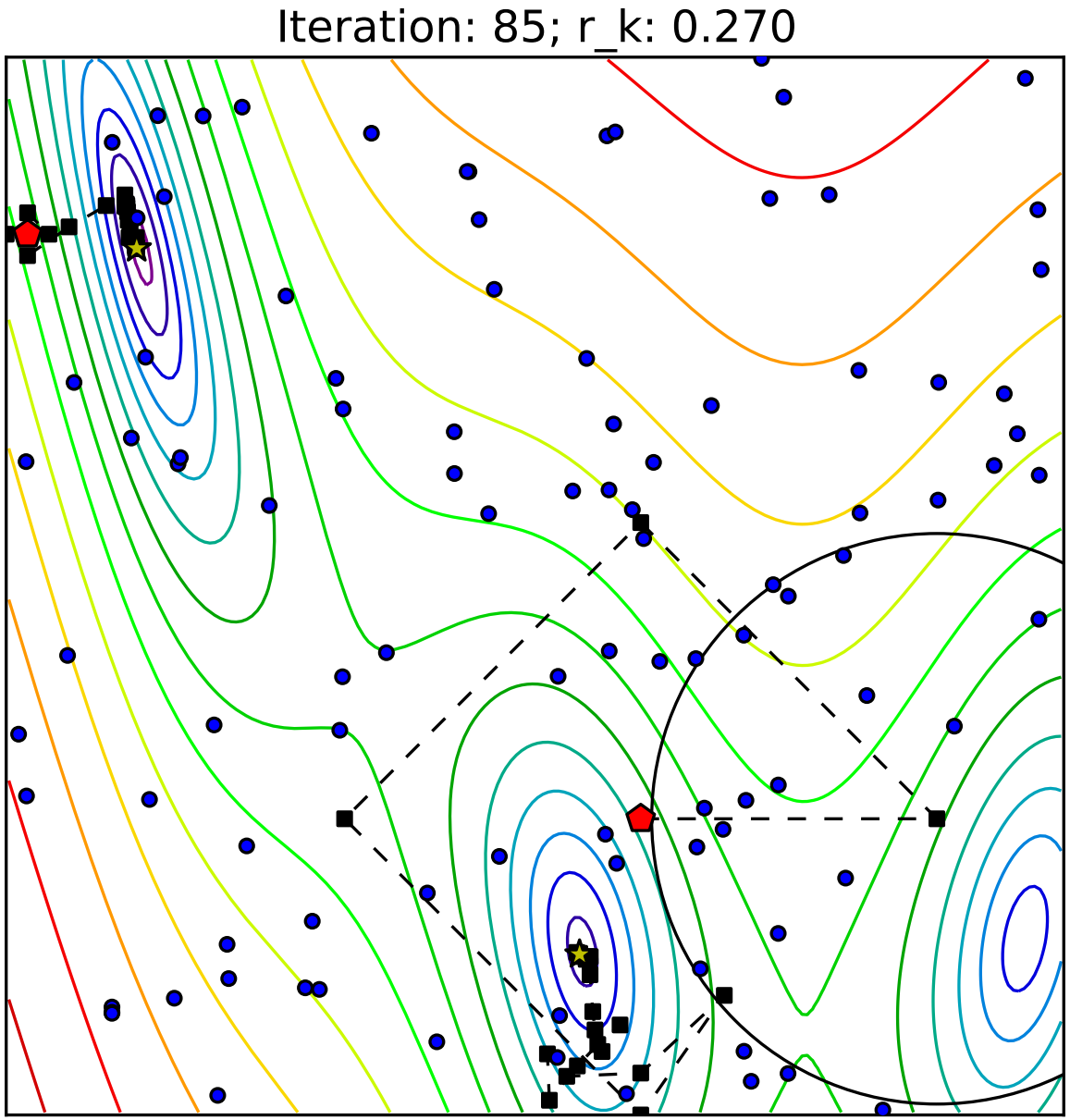

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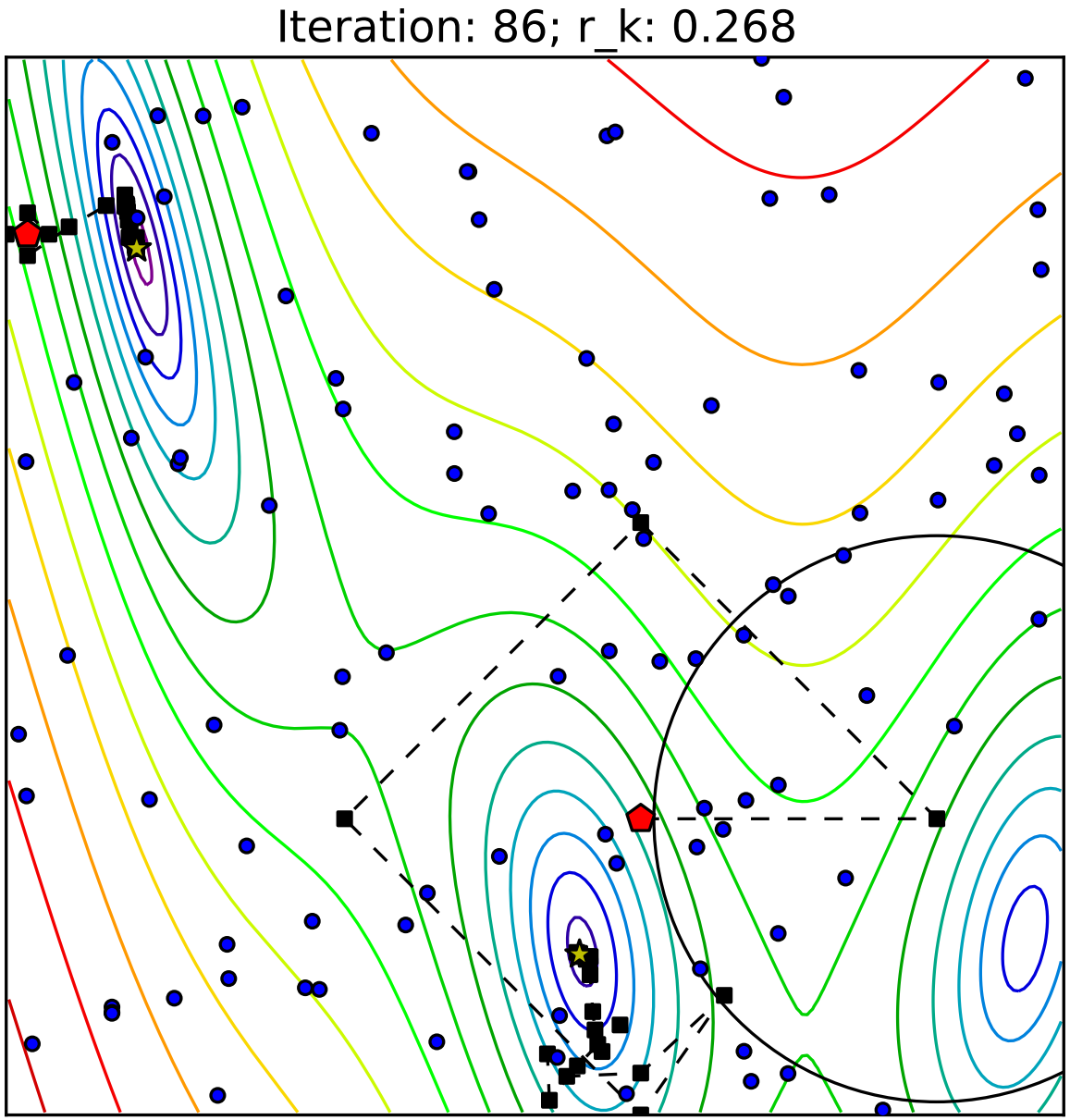

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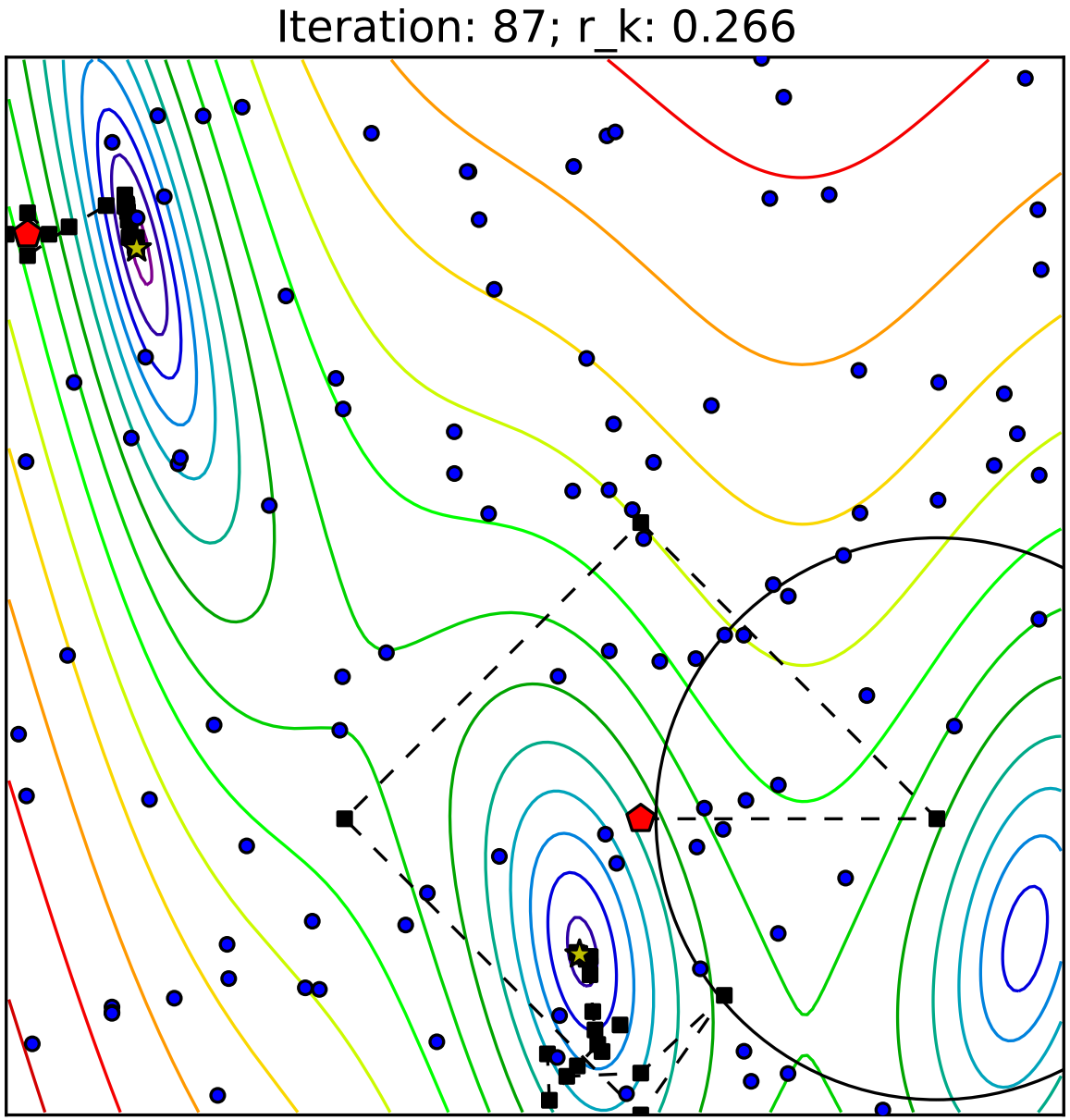

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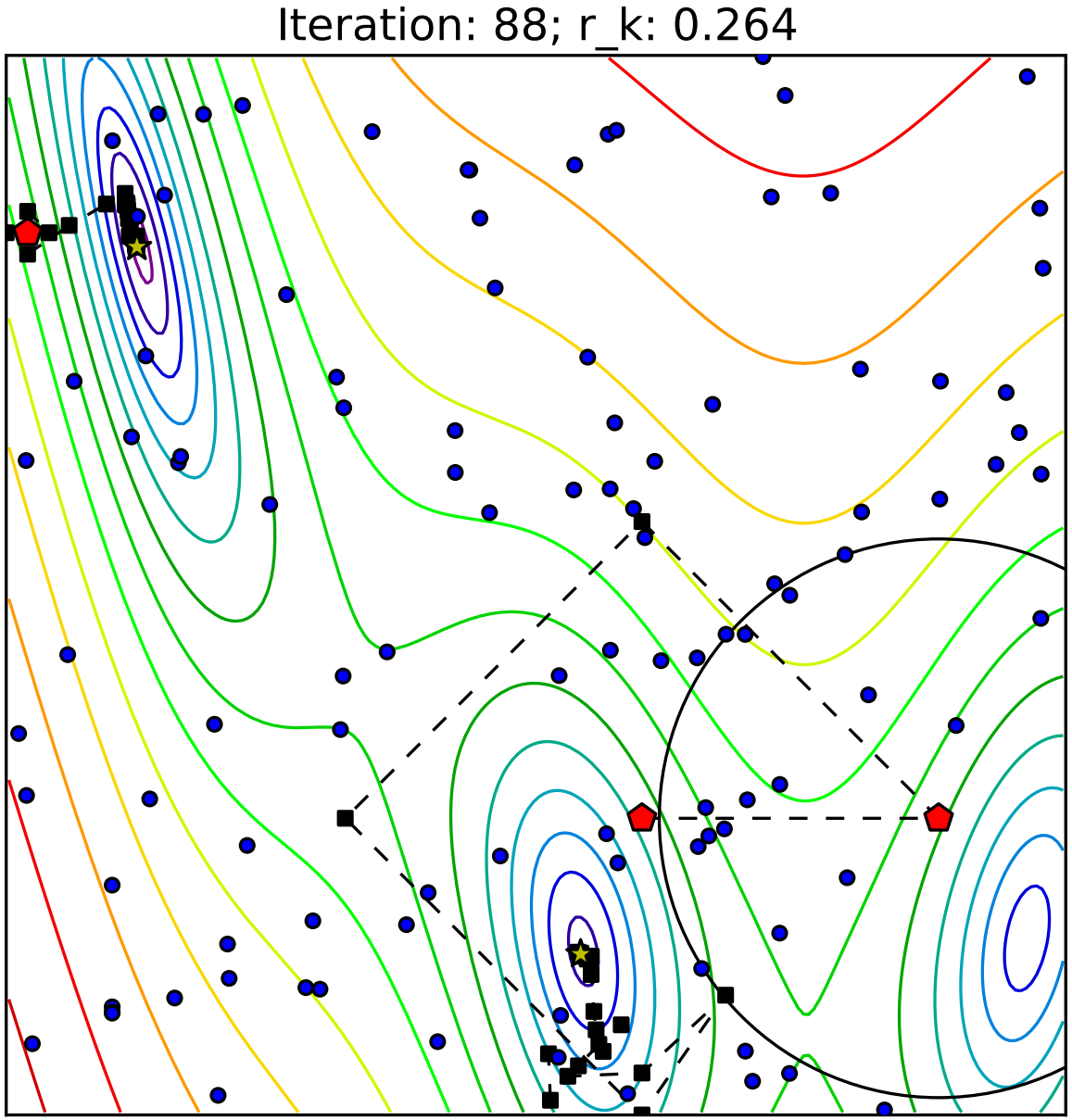

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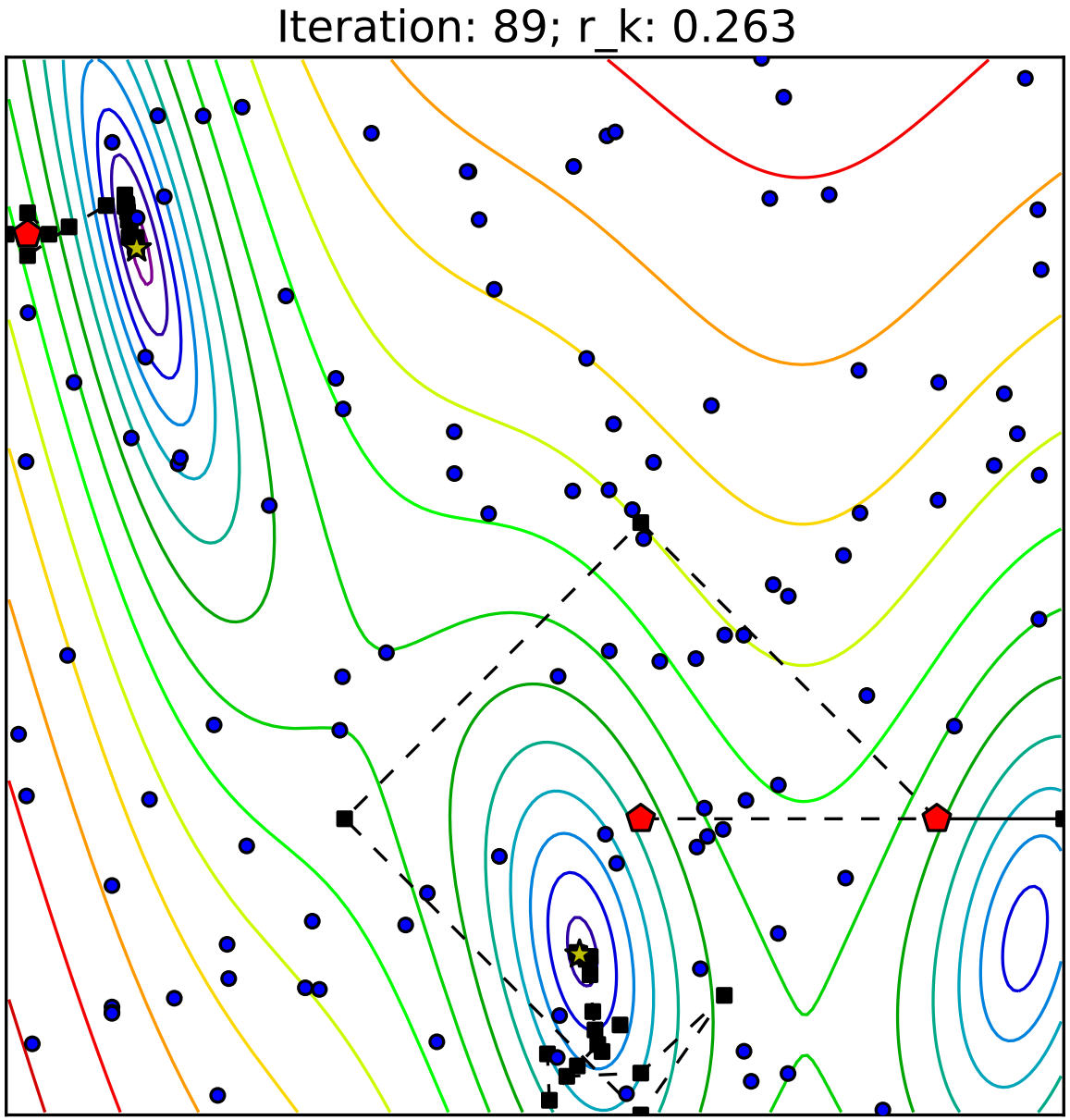

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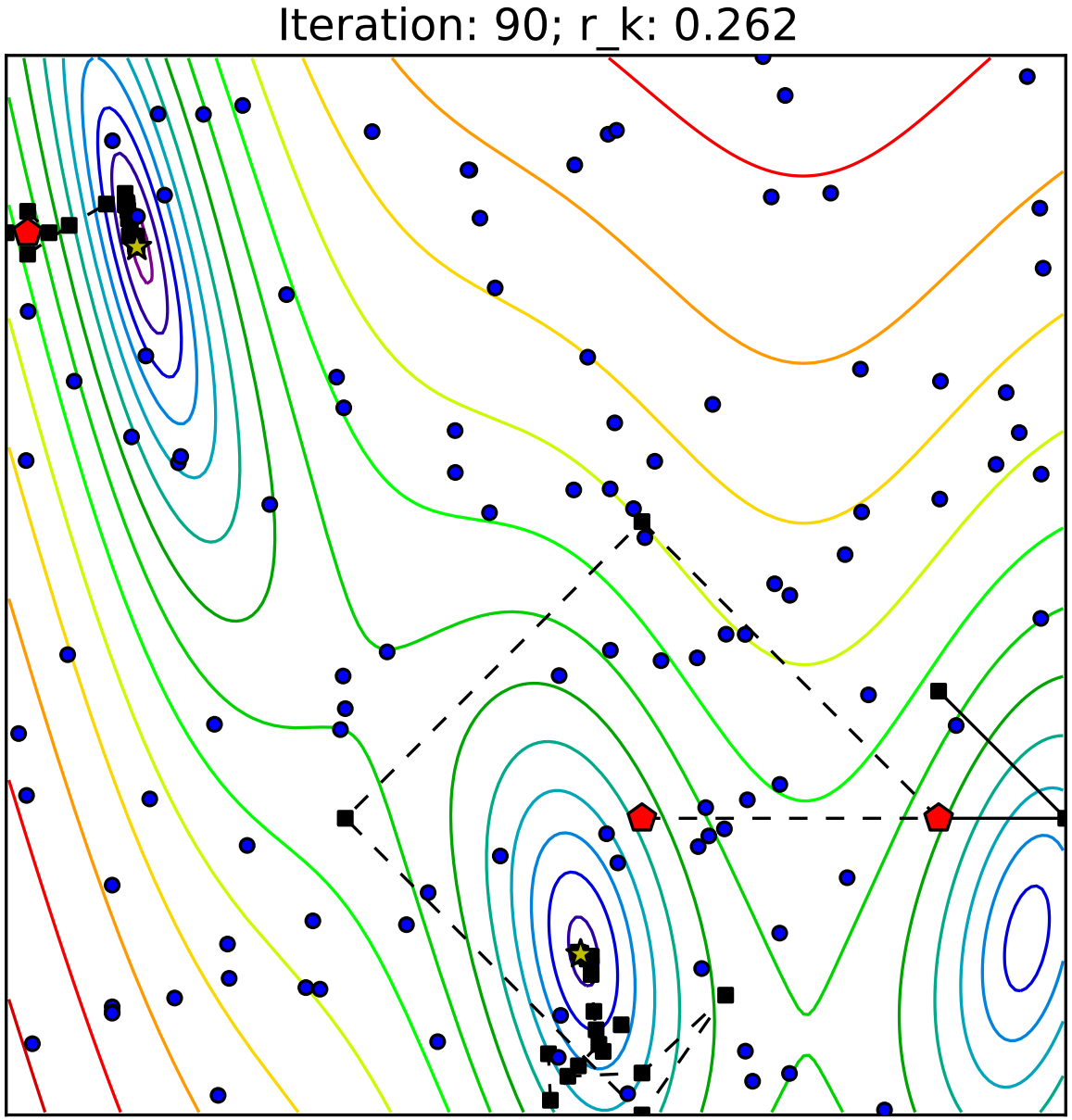

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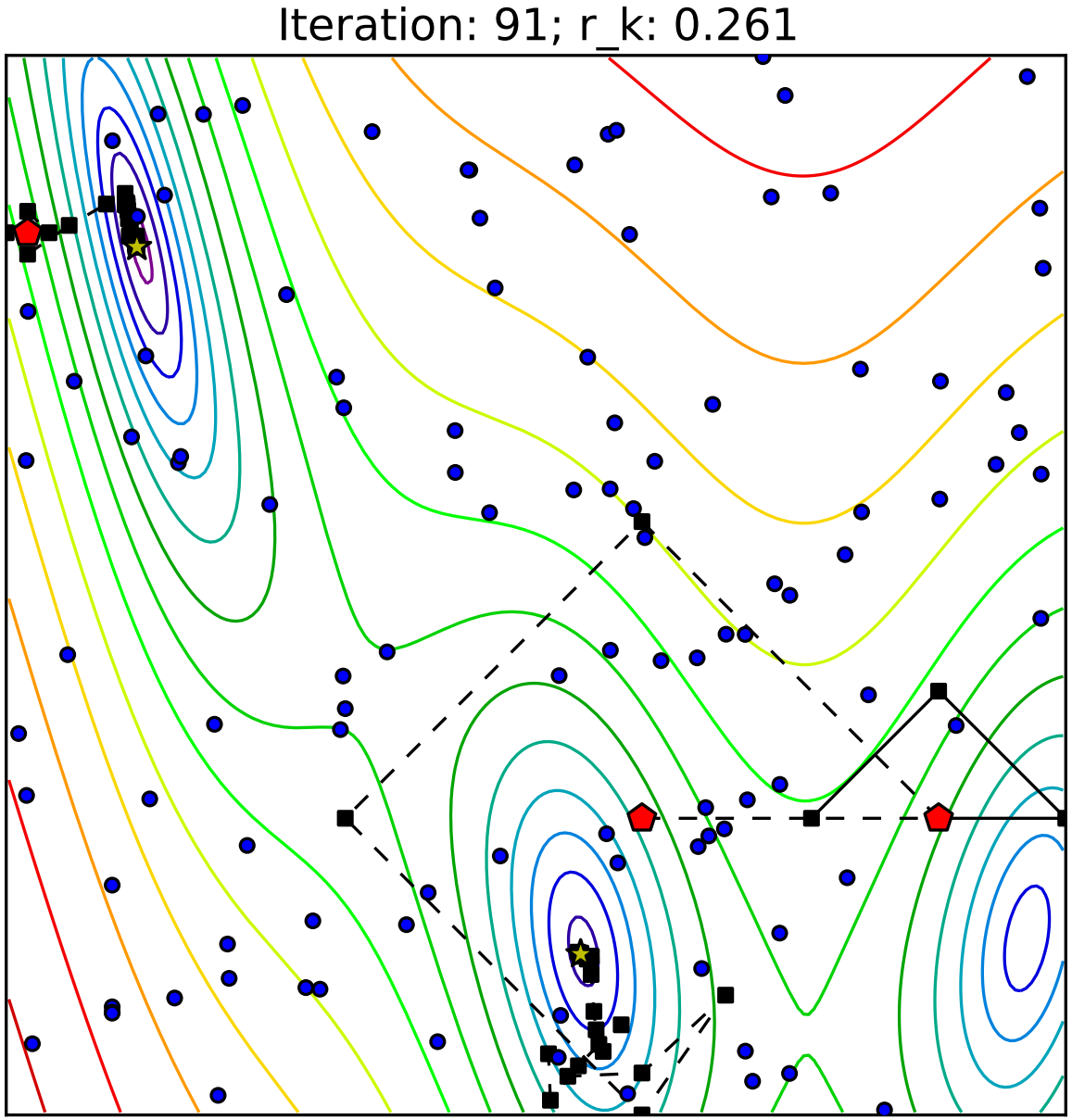

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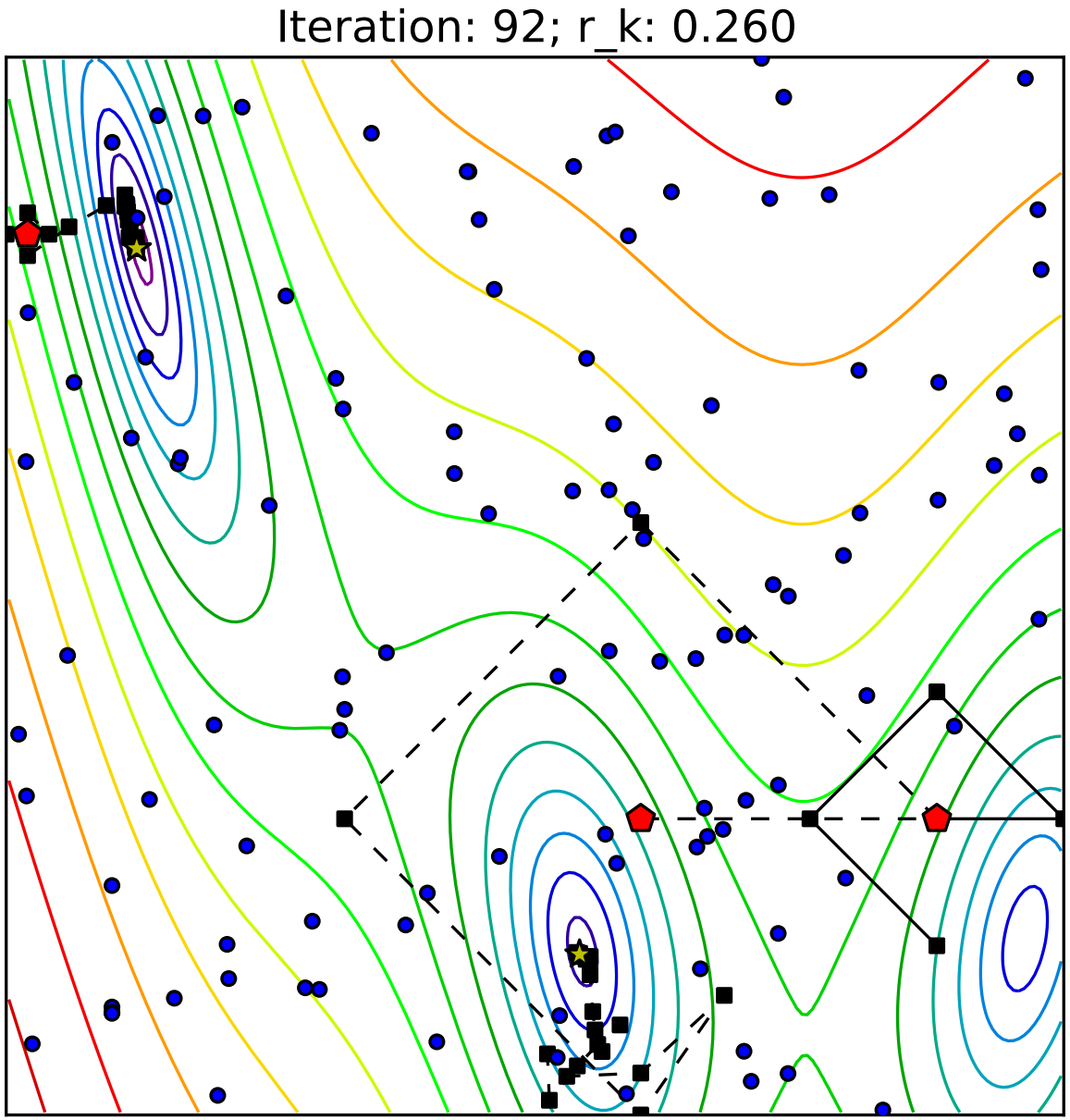

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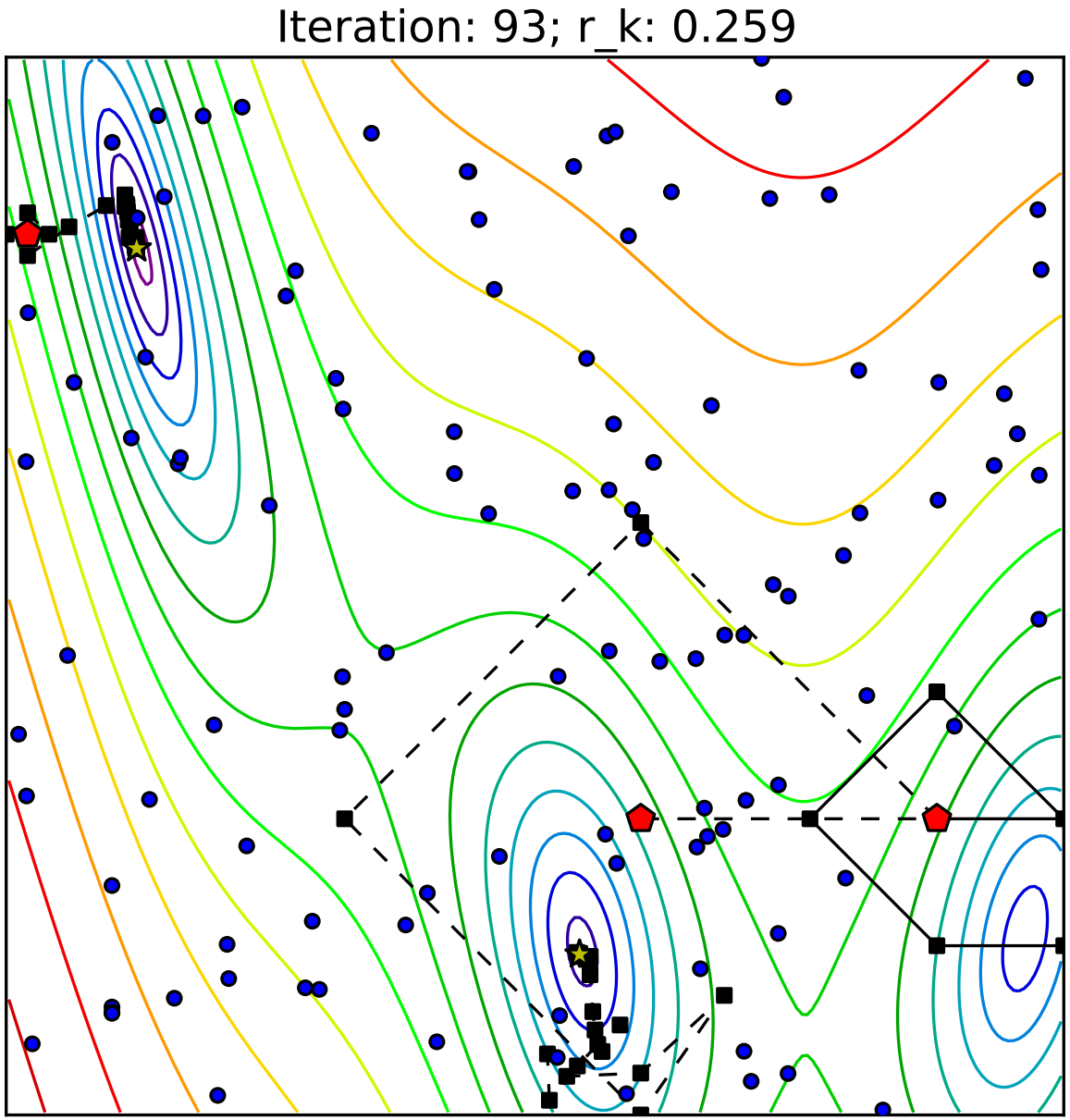

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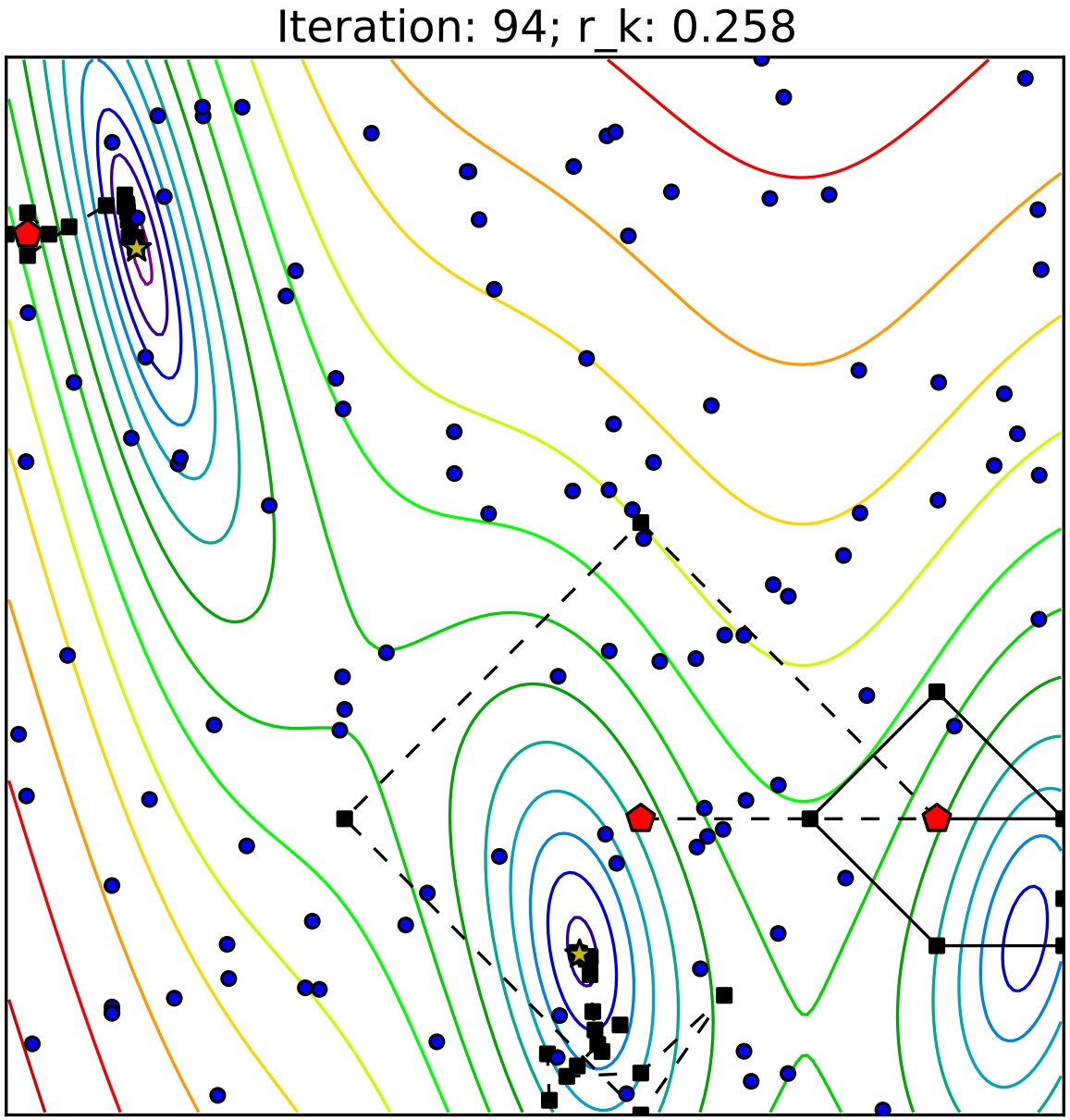

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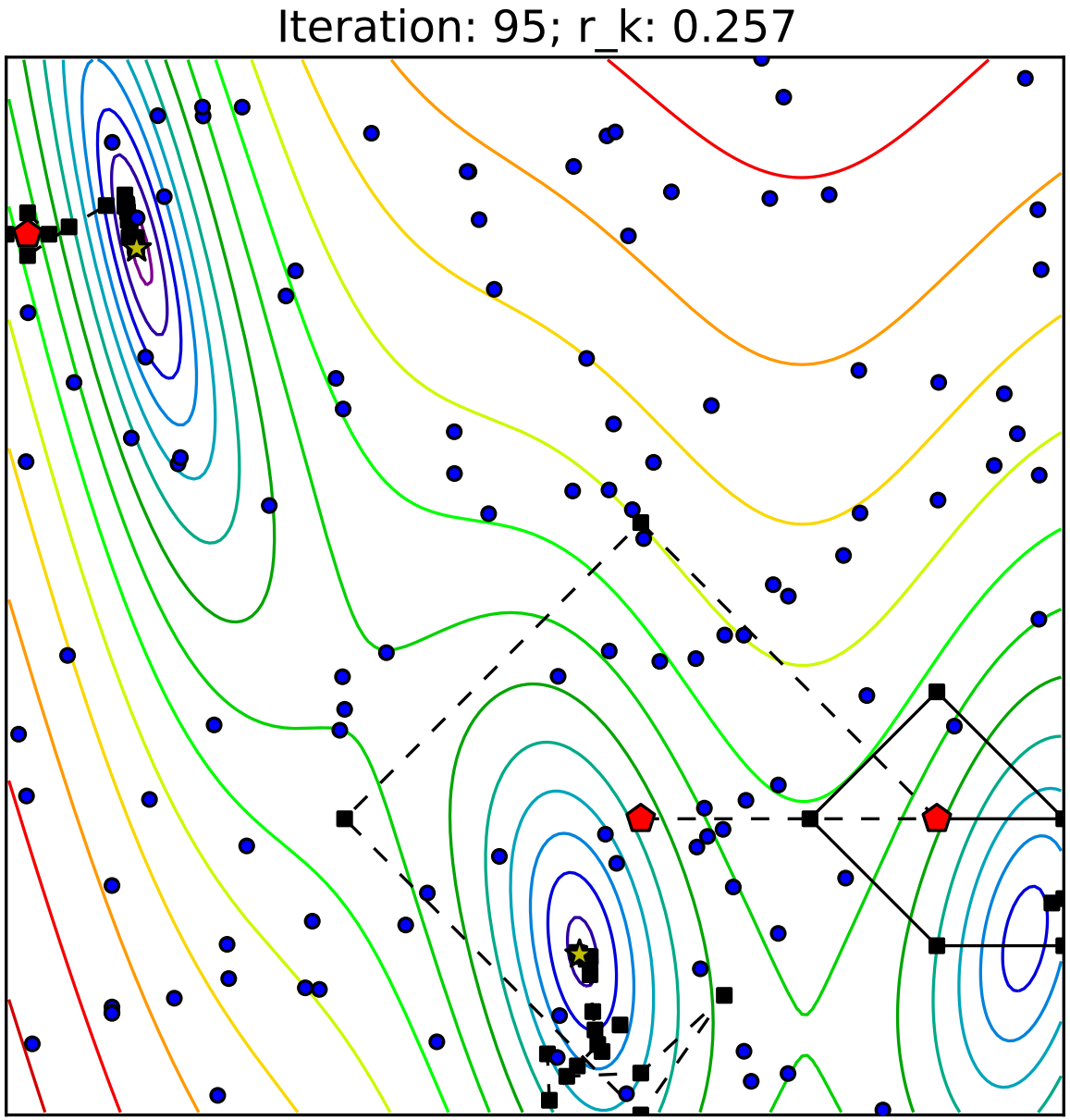

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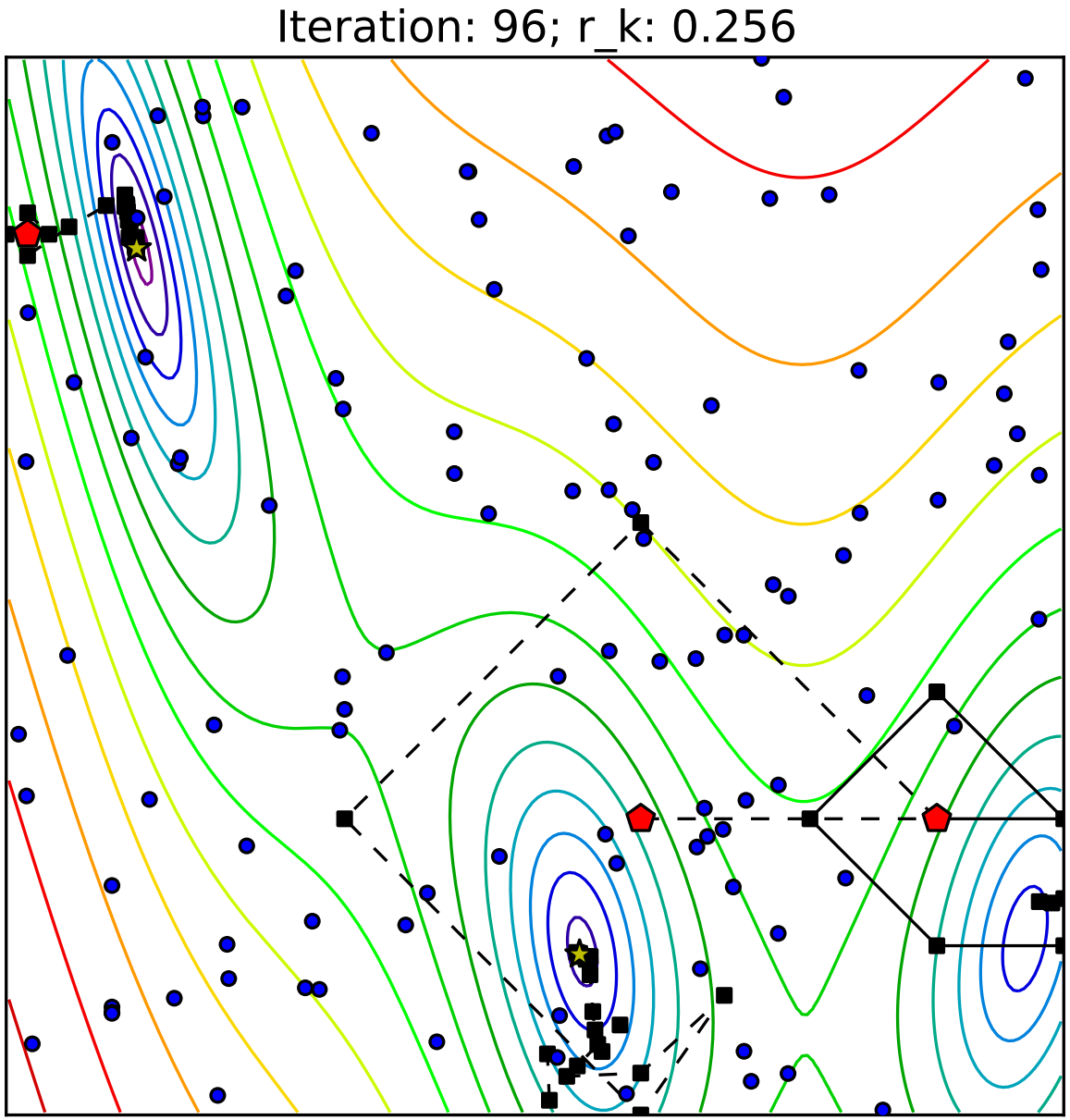

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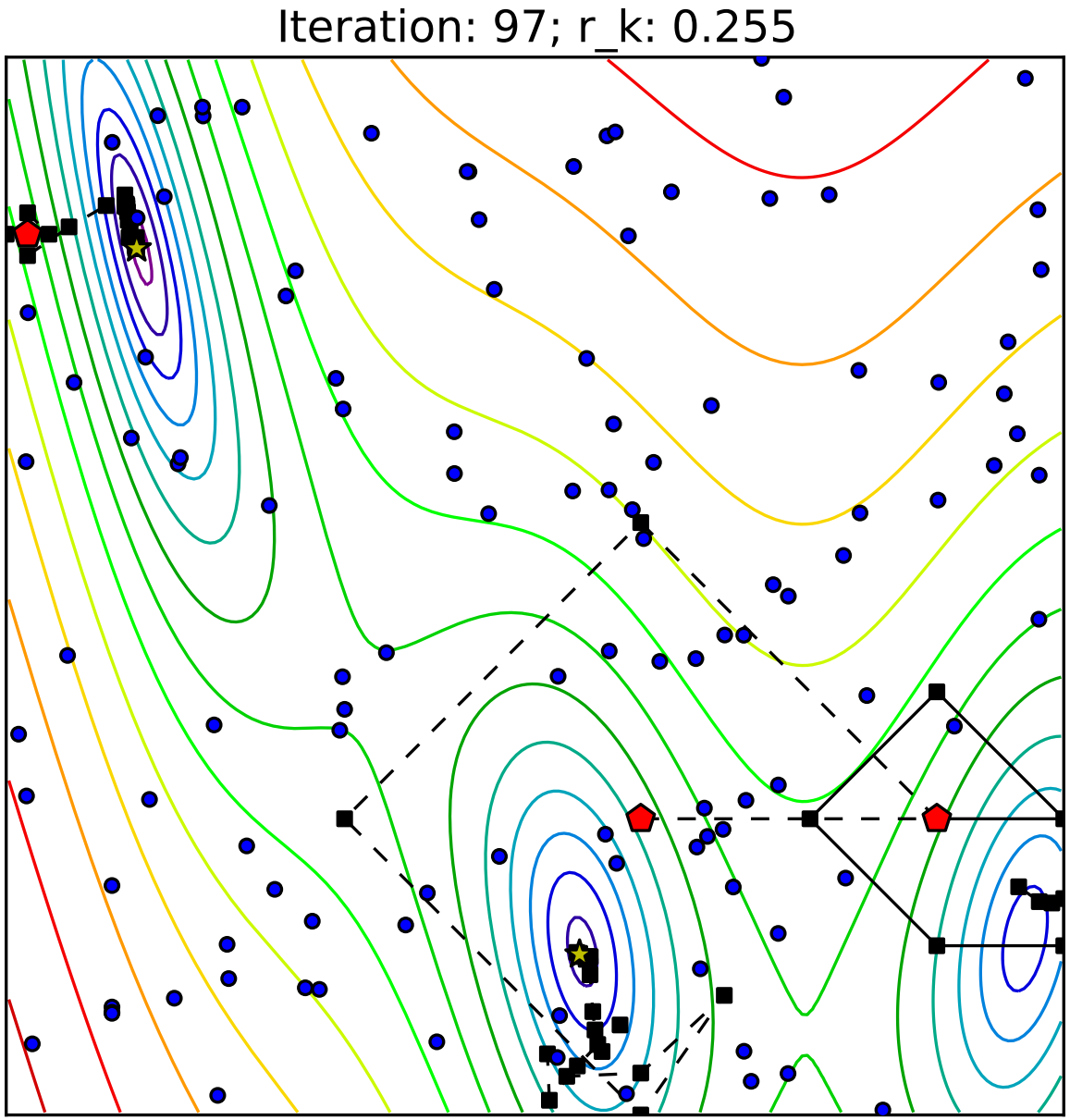

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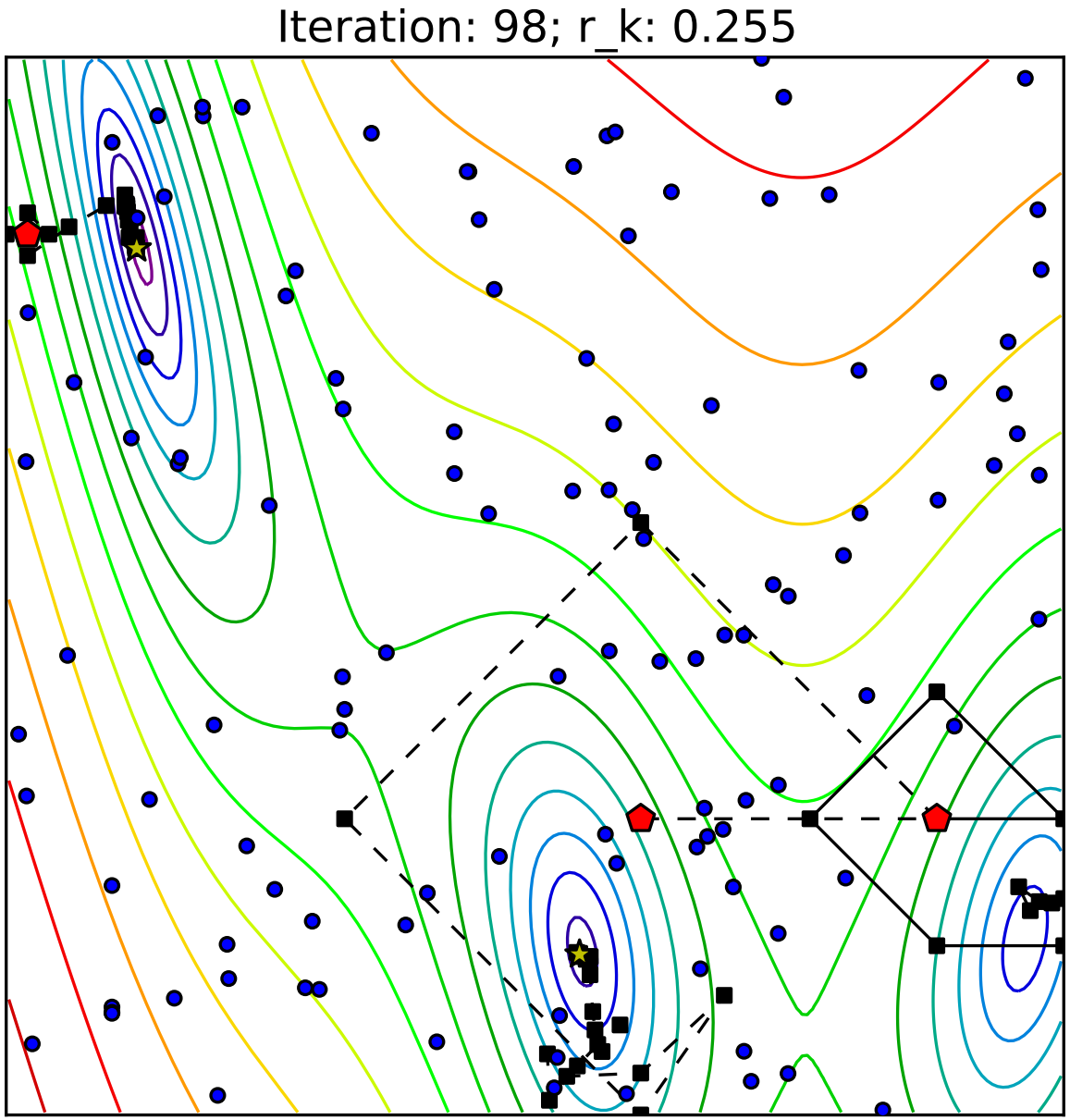

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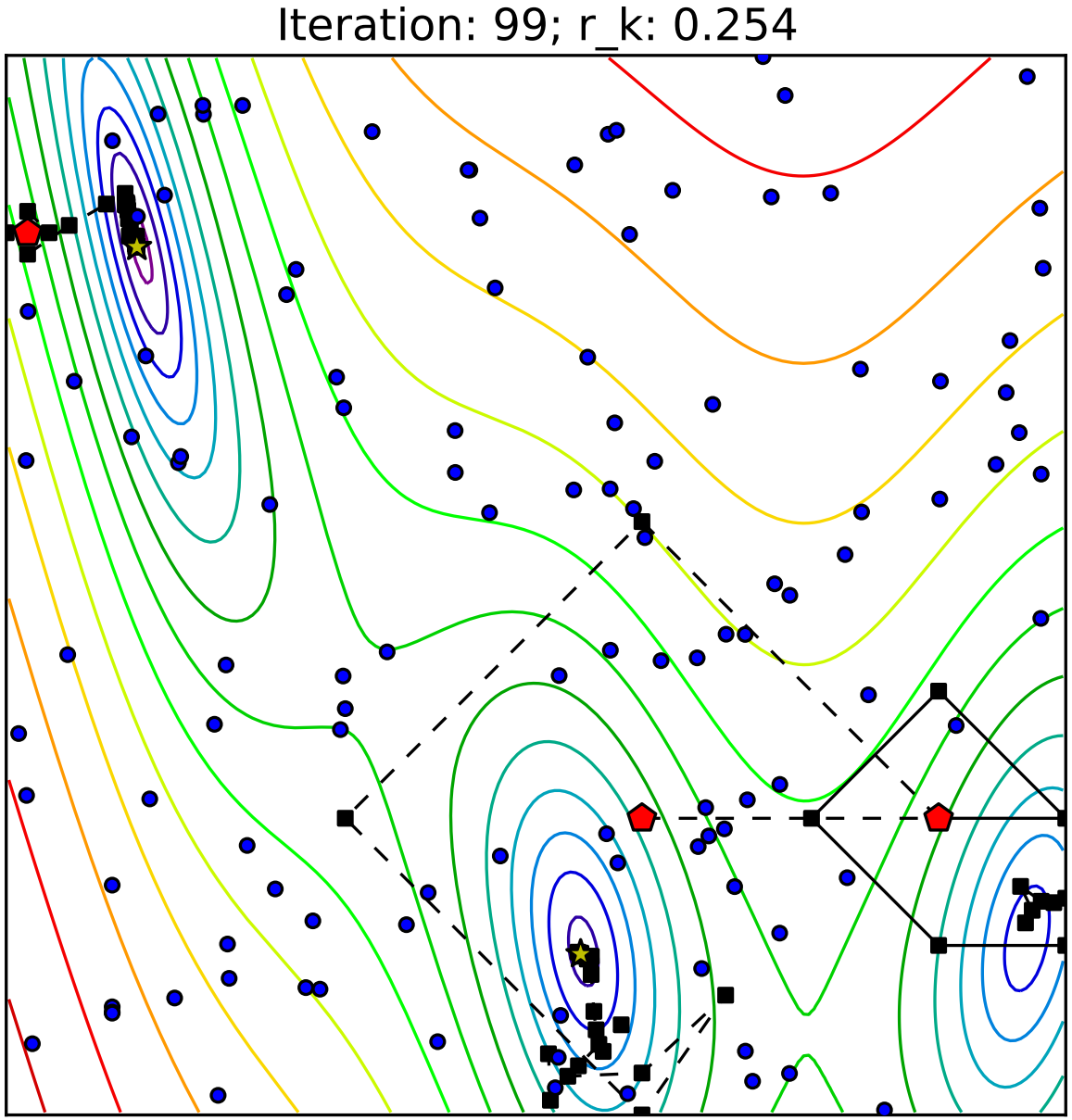

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Possibly beneficial:

- Can return multiple points of interest
- Reports solution quality/confidence at every iteration
- Can avoid certain regions in the domain
- Uses a history of past evaluations of f
- Uses additional points mid-run

Exploiting Structure

- Nonsmooth, composite optimization

$$\underset{x}{\text{minimize}}\, f(x) = h(F(x))$$

  where ∇F is unavailable but ∂h is known

- Least-squares minimization

$$\underset{x}{\text{minimize}}\, f(x) = \sum_i (F_i(x) - T_i)^2$$

Theoretical results

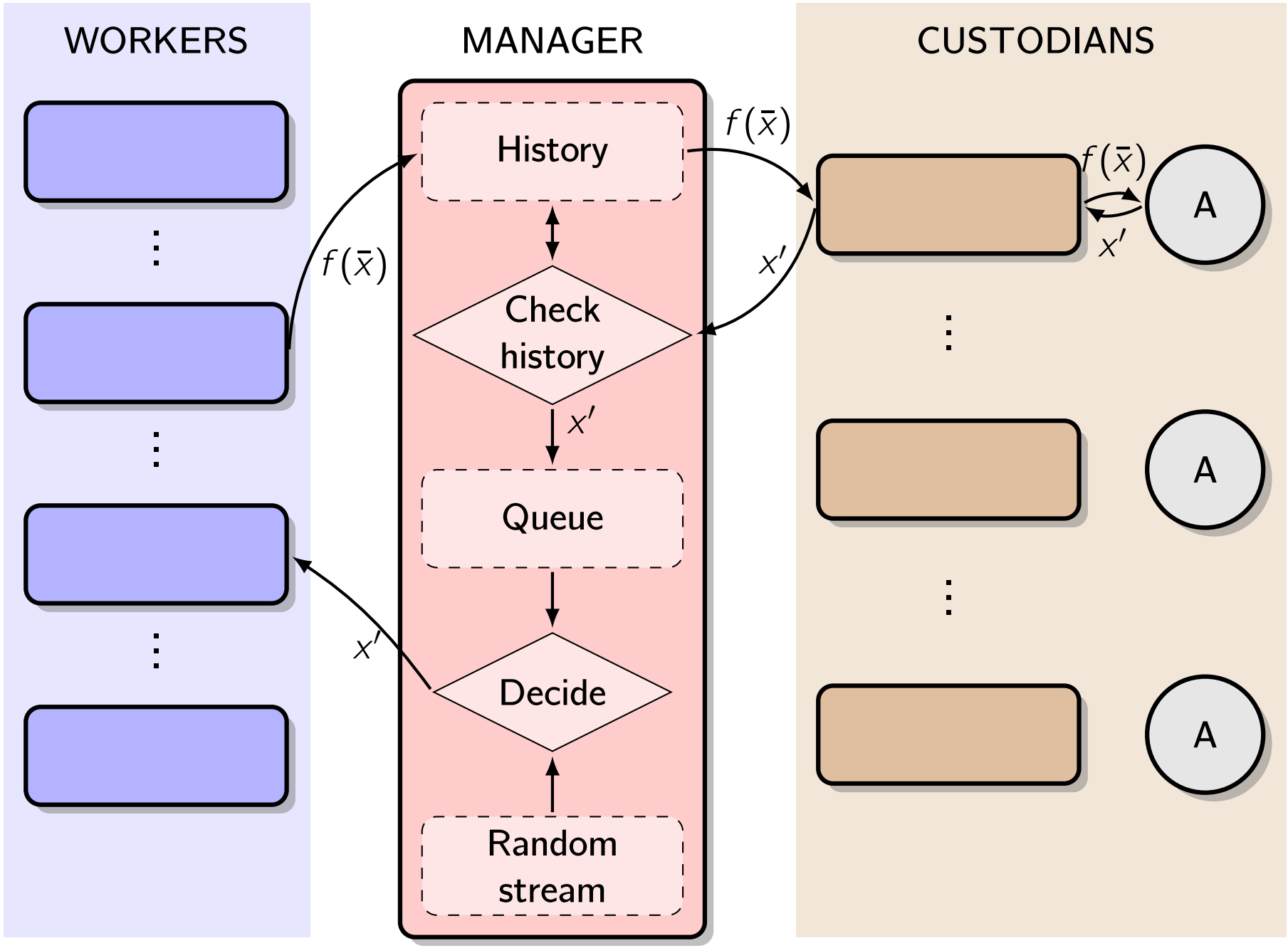
- $f \in C^2$, with local minima in the interior of $\mathcal{D}$, and the distance between minima is bounded away from zero.
- $\mathcal{L}$ is strictly descent and converges to a minimum (not a stationary point).
- Each run has points evaluated often enough
- $$r_k = \frac{1}{\sqrt{\pi}} \sqrt[n]{\Gamma\left(1 + \frac{n}{2}\right) \operatorname{vol}(\mathcal{D}) \frac{5 \log |\mathcal{S}_k|}{|\mathcal{S}_k|}}$$

Theoretical results

- $f \in C^2$, with local minima in the interior of $\mathcal{D}$, and the distance between minima is bounded away from zero.
- $\mathcal{L}$ is strictly descent and converges to a minimum (not a stationary point).
- Each run has points evaluated often enough
- $$r_k = \frac{1}{\sqrt{\pi}} \sqrt[n]{\Gamma\left(1 + \frac{n}{2}\right) \operatorname{vol}(\mathcal{D}) \frac{5 \log |\mathcal{S}_k|}{|\mathcal{S}_k|}}$$

Theorem

Each minima will almost surely be identified: either found in a finite number of evaluations or have a single local optimization run converging asymptotically to it.

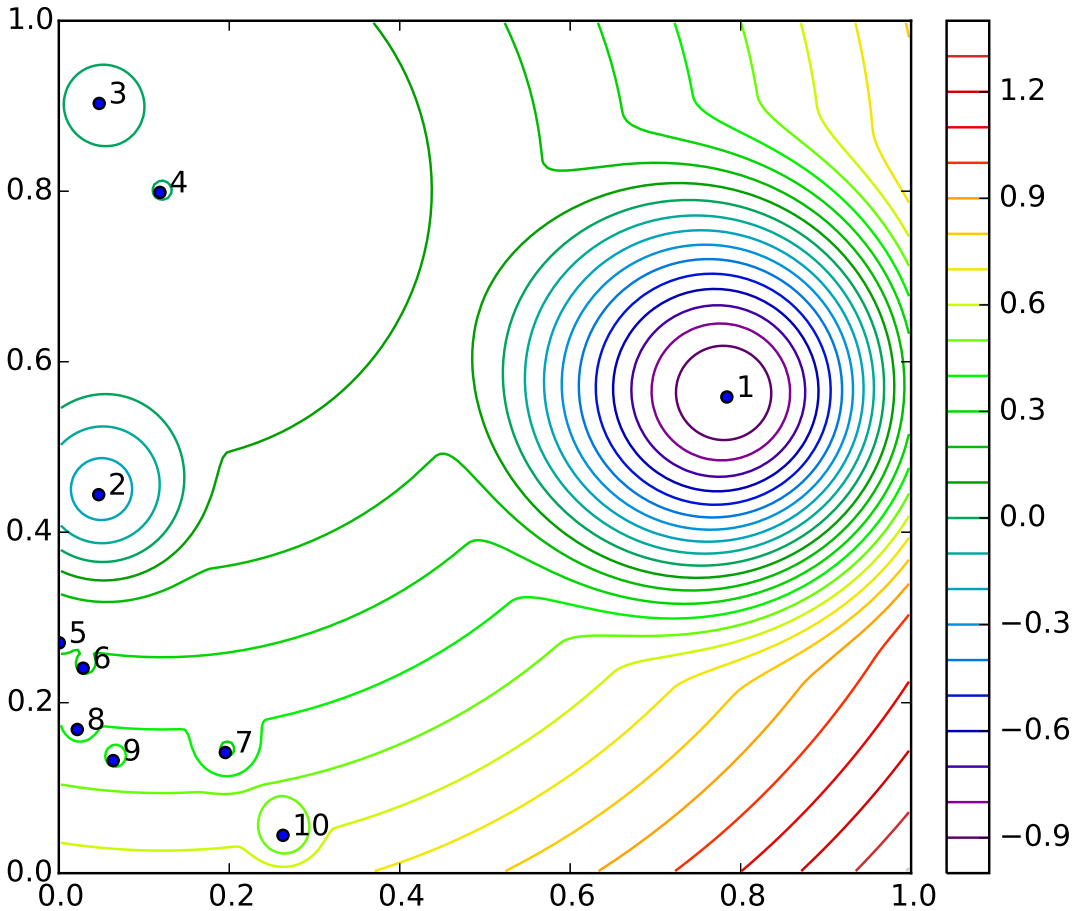

WORKERS
MANAGER
CUSTODIANS
History
Check history
Queue
Decide
Random stream
$f(\bar{x})$
x'
A

Measuring Performance

GLODS	Global & local optimization using direct search [Custódio, Madeira (JOGO, 2014)]
Direct	Serial Matlab DiRect code [Finkel (2003)]
pVTdirect	Parallel DiRect code [He, Watson, Sosonkina (TOMS, 2009)]
CMA-ES	Parallel Covariance Matrix Adaptation Evolution Strategy code [Hansen & Ostermeier (EvolComp, 2001)]
Random	Uniform sampling (as a baseline)
(A)POSMM	[Larson, W. (2016)] with local solver BOBYQA [Powell (2009)], Initial sample size: $10n$

GKLS problems [Gaviano et al., "Algorithm 829" (TOMS, 2003)]

- Smooth augmentation of a convex quadratic; $n = 2, \ldots, 7$
- 10 local minima in the unit cube with a unique global minimum
- 100 problems for each n; 5 replications; $2000(n+1)$ evaluations



Measuring Performance

Notation:

Let X^* be the set of all local minima of f.
Let $f^*_{(i)}$ be the ith smallest value $\{f(x^*)|x^* \in X^*\}$.
Let $x^*_{(i)}$ be the element of X^* corresponding to the value $f^*_{(i)}$.

The global minimum has been found at a level $\tau > 0$ after k evaluations if an algorithm it has found a point $\hat{x}$ satisfying:

$$f(\hat{x}) - f^*_{(1)} \leq (1 - \tau)\left(f(x_0) - f^*_{(1)}\right),$$

where x_0 is the starting point for problem p.

Measuring Performance

Notation:

Let X^* be the set of all local minima of f.
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The j best local minima have been found at a level $\tau > 0$ after k evaluations if:

$$\left|\left\{x^*_{(1)}, \ldots, x^*_{(\underline{j}-1)}\right\} \bigcap \left\{x^*_{(i)} : \exists x \in \mathcal{H}_k \text{ with } \left\|x - x^*_{(i)}\right\| \leq r_n(\tau)\right\}\right| = \underline{j} - 1$$

&

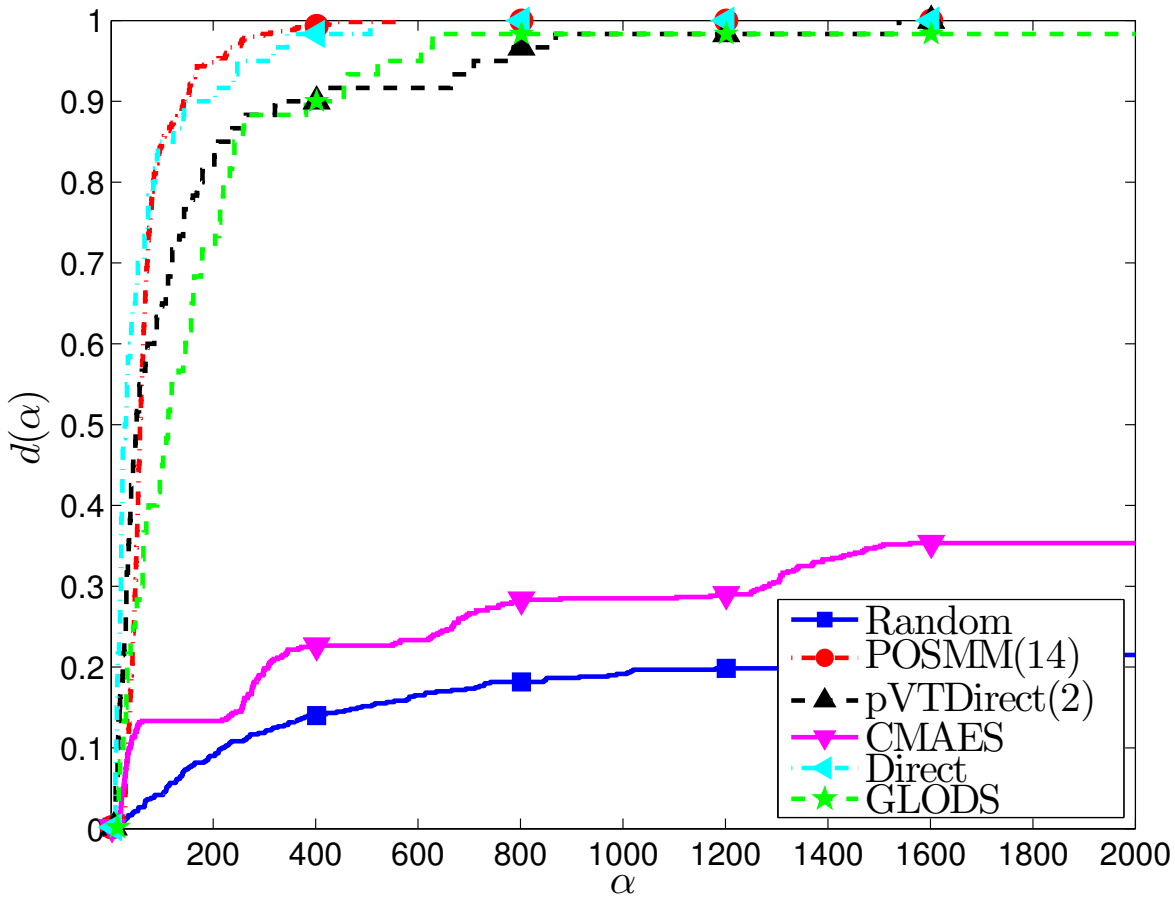
$$\left|\left\{x^*_{(\underline{j})}, \ldots, x^*_{(\bar{j})}\right\} \bigcap \left\{x^*_{(i)} : \exists x \in \mathcal{H}_k \text{ with } \left\|x - x^*_{(i)}\right\| \leq r_n(\tau)\right\}\right| \geq j - \underline{j} + 1,$$

where $\underline{j}$ and $\bar{j}$ are the smallest and largest integers such that $f^*_{(\underline{j})} = f^*_{(j)} = f^*_{(\bar{j})}$ and where $r_n(\tau) = \sqrt[n]{\frac{\tau \, \text{vol}(\mathcal{D})\Gamma(\frac{n}{2}+1)}{\pi^{n/2}}}$.

Ability to Find Approximate Global Minimizer

(A)POSMM

- Makes rapid progress to f_G
- Outperforms other algorithms *(even while demanding 14-fold concurrency)*



$$\tau = 10^{-2}$$

$$f(x) - f_G \leq (1 - \tau)\left(f(x^0) - f_G\right)$$

Ability to Find Approximate Global Minimizer

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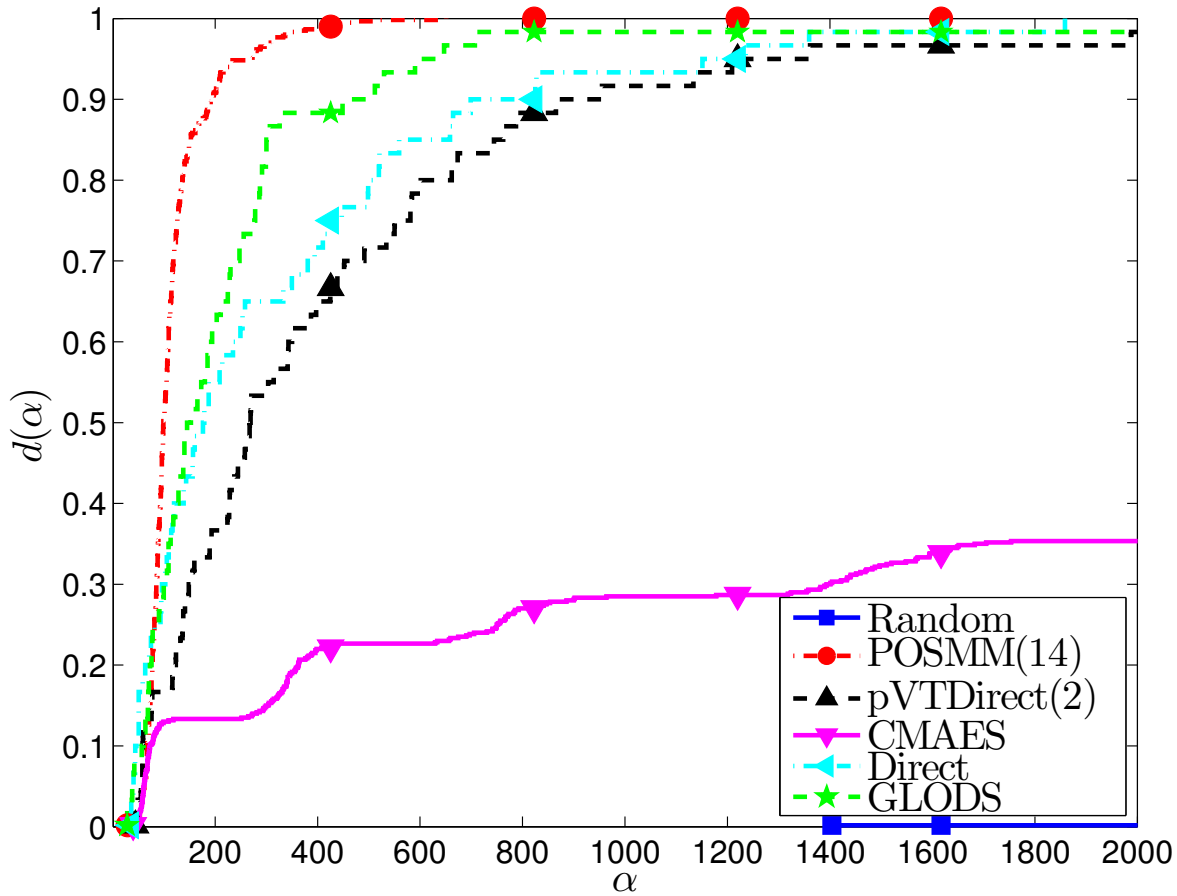
- Outperforms other algorithms *(even while demanding 14-fold concurrency)*



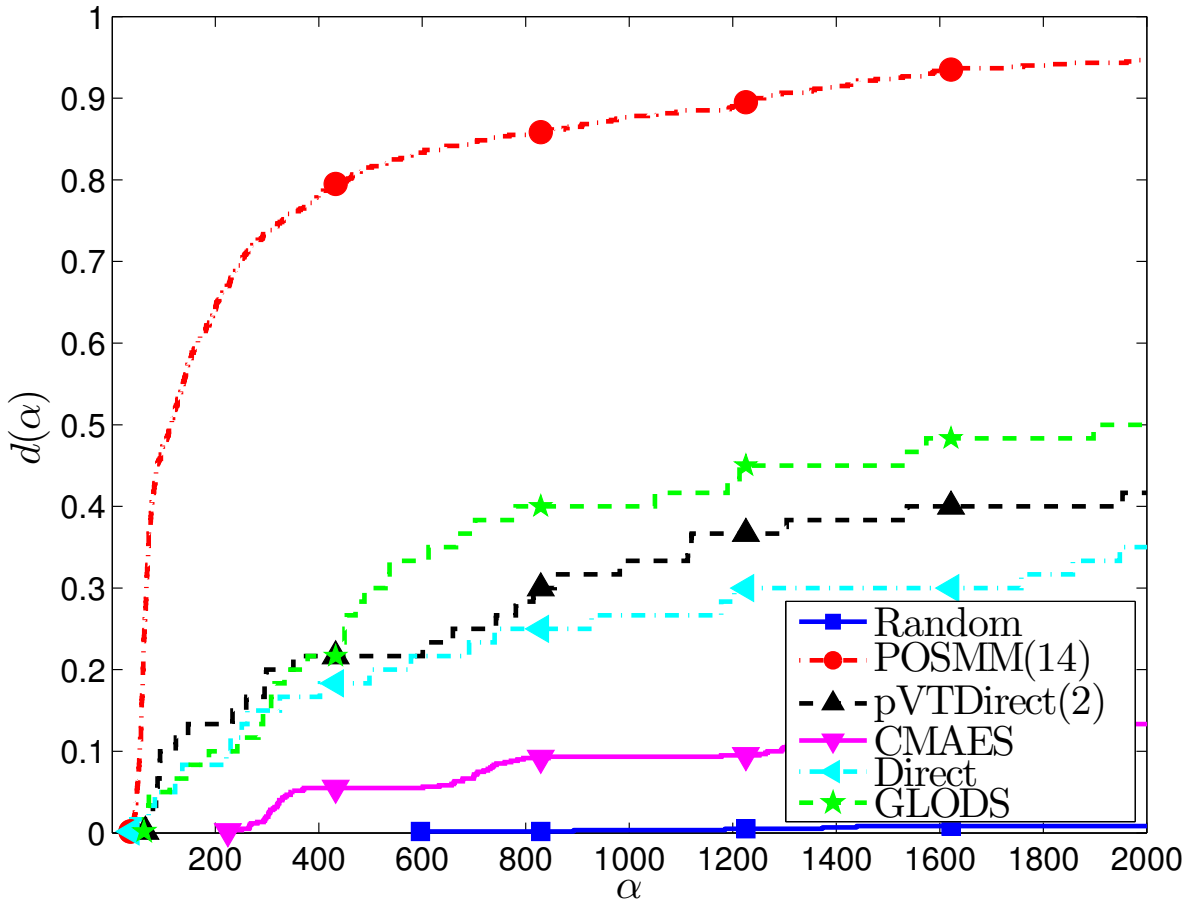
$$\tau = 10^{-5}$$

$$f(x) - f_G \leq (1 - \tau)\left(f(x^0) - f_G\right)$$

Ability to Find j Best Minimizers

(A)POSMM

- Designed to find more than just the global minimizer
- Extends lead for tighter tolerances



distance $\tau = 10^{-5}$, $j = 2$ minimizers

Ability to Find j Best Minimizers

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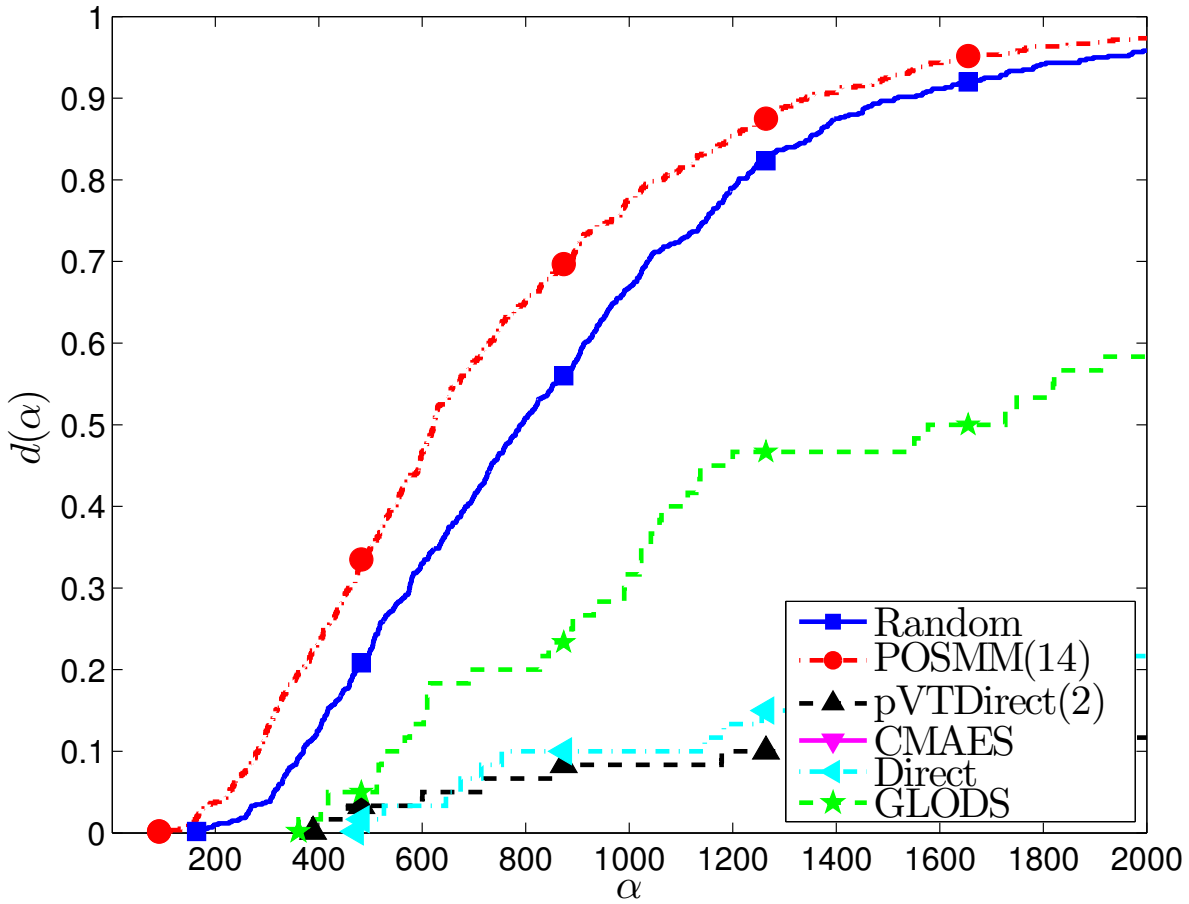

distance $\tau = 10^{-3}$, $j = 7$ minimizers

Ability to Find j Best Minimizers

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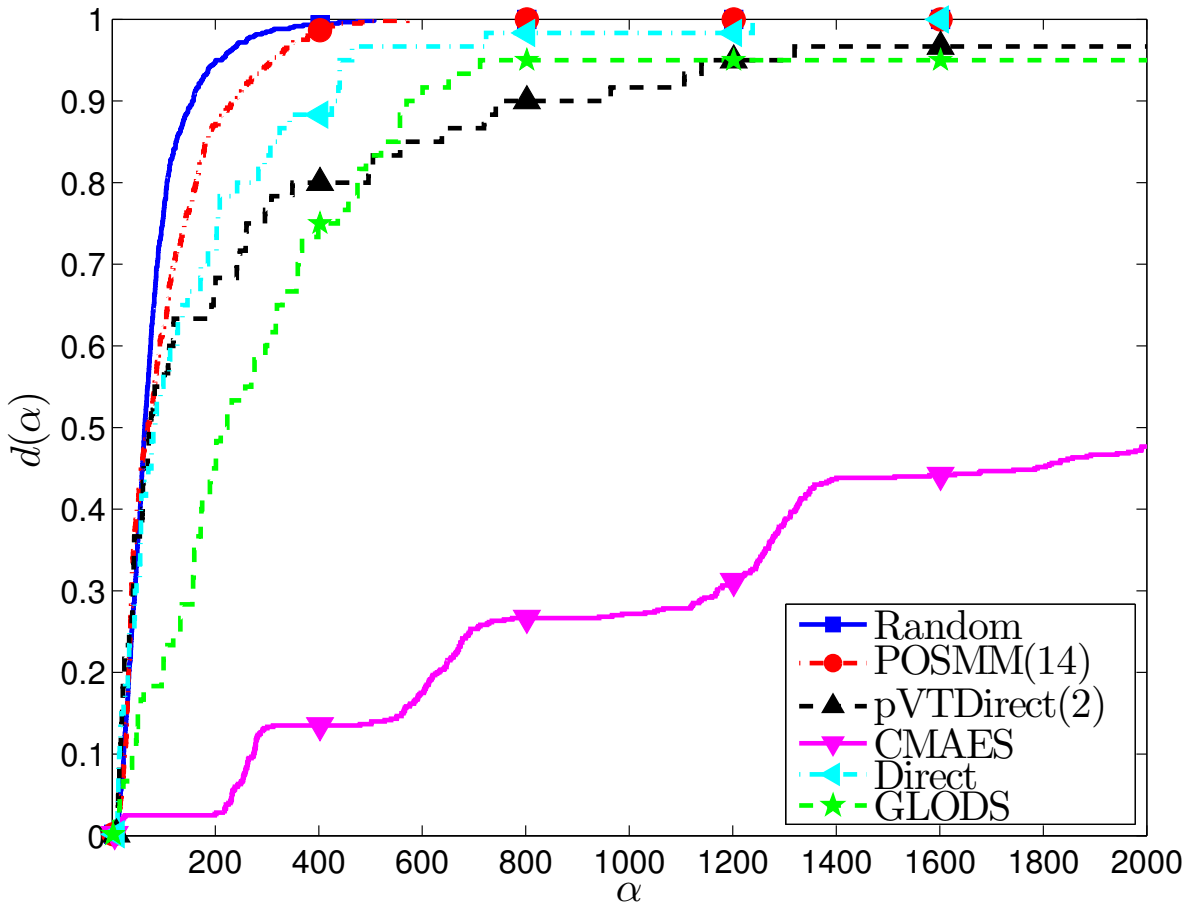

distance $\tau = 10^{-2}$, $j = 3$ minimizers

Ability to Find j Best Minimizers

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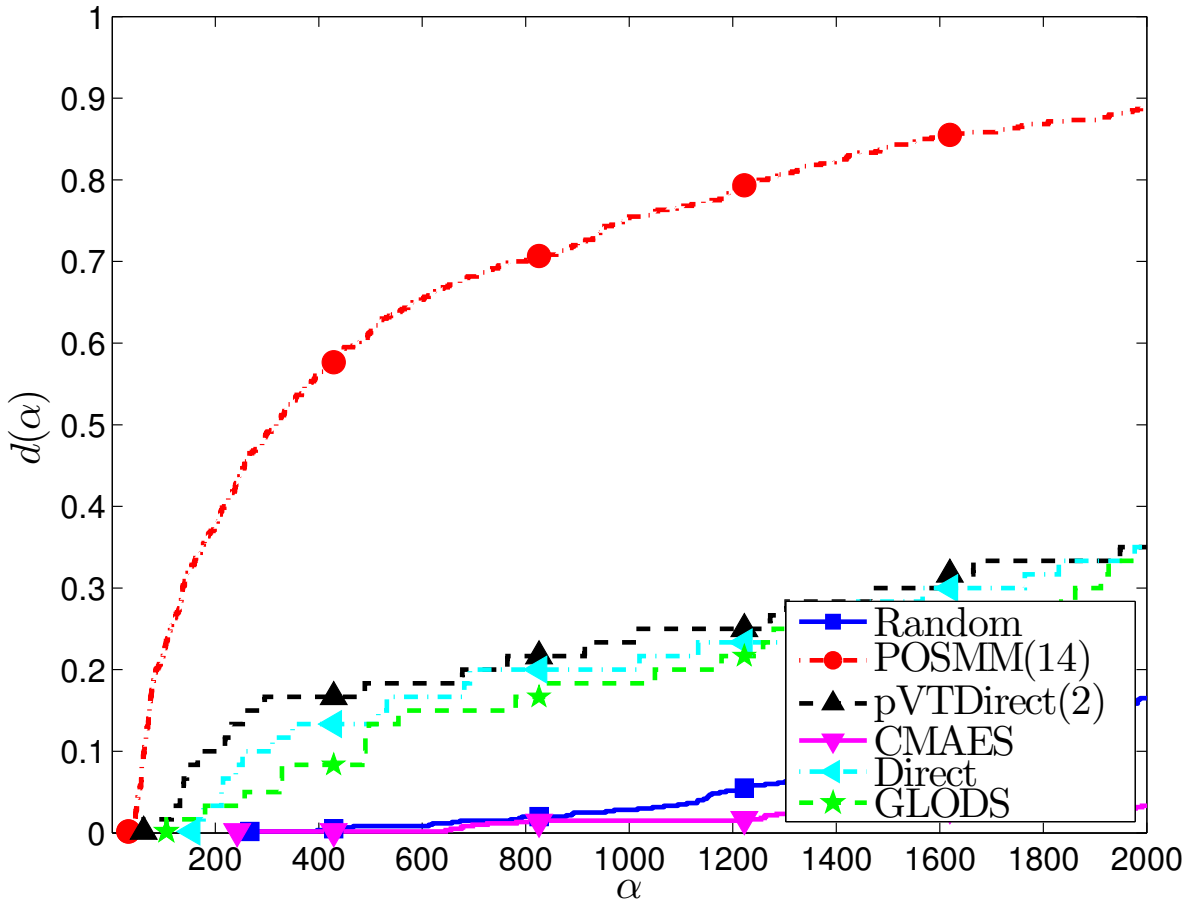
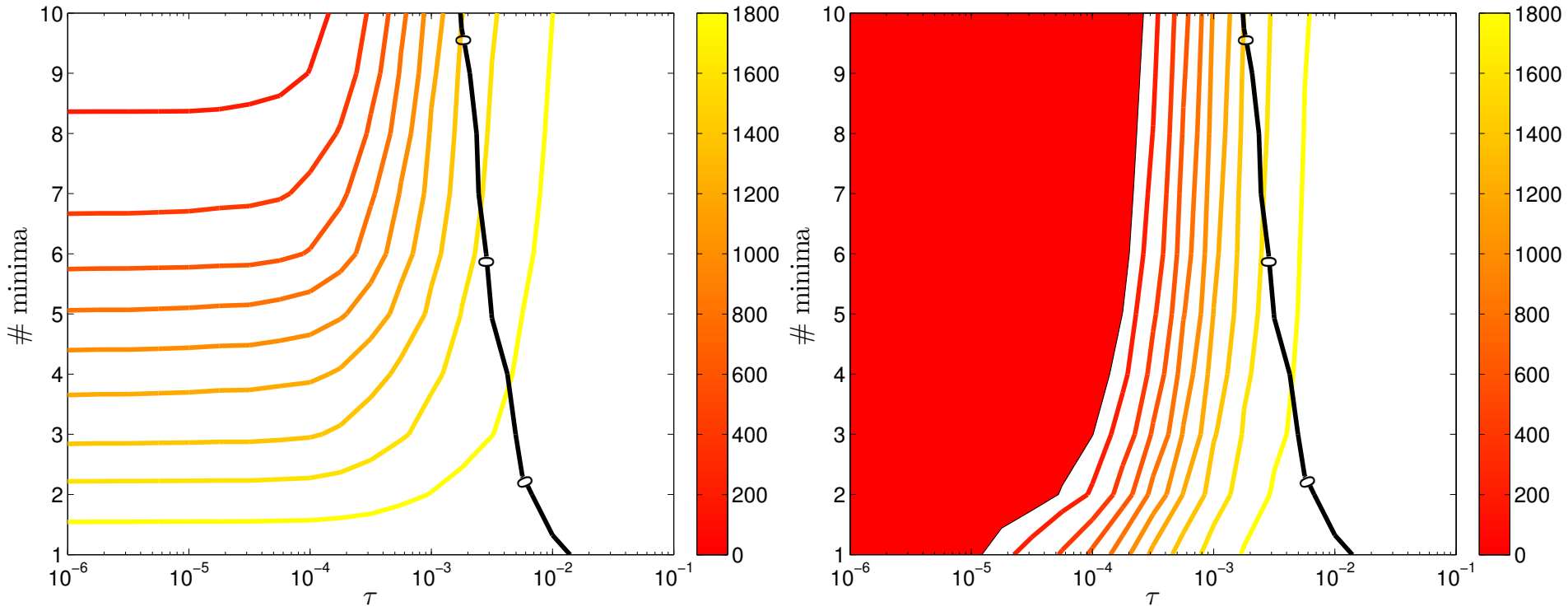


distance $\tau = 10^{-4}$, $j = 3$ minimizers

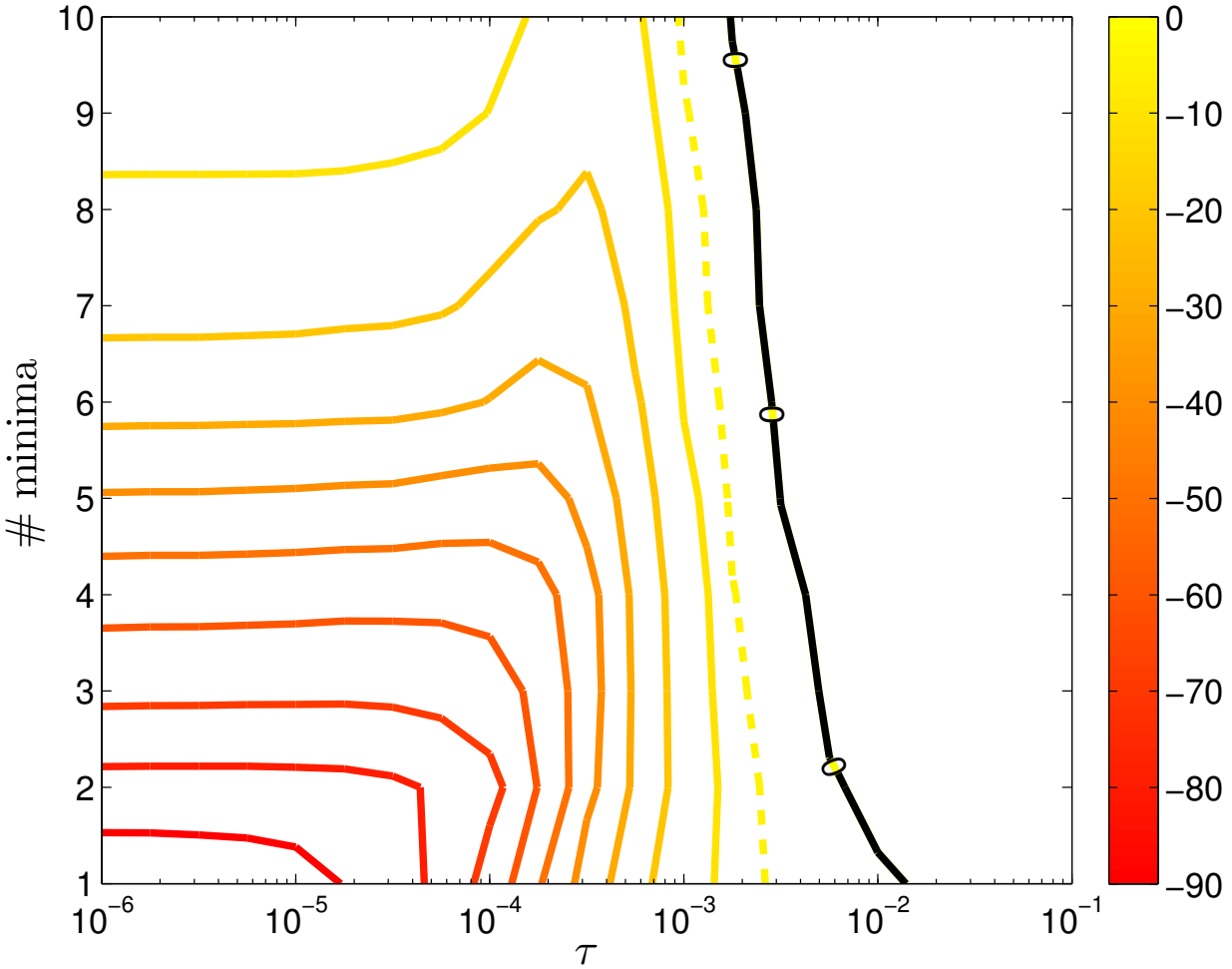
(Tolerance, # Minimizers) Comparison With Random Sampling

Area under data profile: POSMM (L), RS (R)



(Tolerance, # Minimizers) Comparison With Random Sampling

Percent difference between POSMM and RS areas



APOSMM has clear advantages as tolerances tighten

Closing Remarks

- Concurrent function evaluations can locate multiple minima while efficiently finding a global minimum.

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Current work:

- Finding (or designing) the best local solver for our framework
- Best way to process the queue?

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